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NONADIABATIC THEORY OF INELASTIC ELECTRON-HYDROGEN SCATTERING

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Nonadiabatic Theory of Inelastic Electron-Hydrogen Scattering

H. L. Kyle
Goddard Space Flight Center
National Aeronautics and Space Administration
Greenbelt, Maryland

ABSTRACT

A brief history is given of the experimental measurements of the probability for the excitation of atomic hydrogen from the H(1s) state to the H(2s) state by electron impact. It is pointed out that the experiments leave the excitation cross section, σ_{1s-2s} uncertain by as much as a factor of two between 10.2 and 50 eV. The problem is then stated in theoretical terms. A brief description of the close coupling approximation is given and the desirability of an alternate method of approach is pointed point. The nonadiabatic theory is briefly reviewed.

A formalism for the nonadiabatic treatment of the scattering of low energy s-wave electrons from atomic hydrogen is developed, and the zeroth order (angle-independent) approximation is explicitly solved. The zeroth order approximation for the excitation of the 2s level from the ground state is described by the same equation used to describe elastic scattering below

the 2s threshold, but with more complicated boundary conditions. The solution has been effected by expanding the wave function in terms of separable solutions. The cross sections σ_{1S-2S} and σ_{1S-2S} are directly obtained from the calculation. With the assumption of reciprocity it is also possible to obtain σ_{2S-2S}. The elastic cross sections, σ_{1S-1S}, are within one percent of the close coupling results in the triplet case, but are about 20 percent greater in the singlet case. The inelastic cross sections, σ_{1S-2S}, are reduced about 20 percent in the triplet case and 20 percent to 40 percent in the singlet case relative to the close coupling results. AUTHOR

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INTRODUCTION

Within the last few years there has been a great renewal of interest in the problem of the scattering of electrons with kinetic energy less than 100 eV from atomic hydrogen. The problem is of interest as a basic problem of quantum mechanics while the resulting cross sections are greatly desired by those studying stellar atmospheres and interplanetary and interstellar space where atomic hydrogen predominates. The upsurge in interest was started by the possibility of using fast electronic computers to solve problems whose solution had previously been too laborious; it was helped along by the tremendous growth of interest in the exploration of the solar system during the last decade; and was given a final push by the development of experimental methods which allowed certain of the scattering and excitation cross sections to be measured in the laboratory.

This paper is an attempt to expand the nonadiabatic scattering theory, Temkin (1960, 1962A), to include inelastic scattering phenomena. This will provide an alternate, and it is hoped more accurate procedure, to the close coupling methods, Burke and Smith (1962). As shown later it may also shed some light on the accuracy of the close-coupling technique. In particular the inelastic S-wave scattering of low energy electrons from atomic hydrogen will be treated and the probability of exciting the target atom from the H(1s) to the H(2s) state calculated. As side products the elastic scattering cross sections $\sigma_{1s\to 1s}$ and $\sigma_{2s\to 2s}$ will also be obtained.

CHAPTER I

History of the Problem

1. Experimental

The laboratory measurements of the $\sigma_{1s\rightarrow 2s}$ cross sections are of basic importance to this thesis and will be briefly discussed. The experimental ground work was laid by Lamb and Retherford (1950, 1951). In fact they obtained some evidence as to the energy dependent shape of the $\sigma_{1s\rightarrow 2s}$ curve near threshold from measurements taken during their investigation of the fine structure of the n = 2 states of H. However, the first determined effort to measure the cross section was made by Lichten and Schultz (1959). They measured $\sigma_{1s\rightarrow 2s}$ from 10.2 eV (threshold) to about 45 eV.

A brief description of the Lichten and Schultz experiment is in order. Molecular hydrogen at a pressure of 2 mm was heated to 3000° K in a tungsten oven. Under these conditions dissociation is 91 percent complete [Wooley, Scott, and Brickwedde (1948)]. A collimated beam of atom hydrogen flowed from the oven into a vacuum chamber where it was crossed at right angles by an electron beam of controlled energy. Atoms excited to the H(2p) state, with lifetimes of the order of 10^{-9}sec, decayed with the emission of Lyman-alpha radiation while still in the collision region. However, atoms excited to the H(2s) are metastable and hence could pass into a third chamber where they were detected. Two methods of detection were used to obtain the 1s-2s cross section. In the first case the relative cross section was

measured by use of a metallic detector from which impinging H(2s) atoms ejected electrons. The scatter of individual measurements at a given energy was small, and hence the energy dependent shape of the excitation cross section could be accurately determined. However, the published absolute cross sections depended upon a normalization of the measurements to the first Born approximation between 30 and 40 eV. The validity of this normalization procedure at such low energies has since been called in question by Hummer and Seaton (1961) and others. Secondly, H(2s) can be quenched by an electric field, which causes mixing of the 2s and 2p states. This considerably accelerates the decay of the H(2s) atoms. The resultant Lyman-alpha radiation can be detected. An absolute measure of the cross section was obtained using the yield of the photon detector, the geometry of the apparatus, and the known conditions of the source and electron gun [Lichten and Schultz (1959)]. The method of calculation was taken from Lamb and Retherford (1950). The results in this case were, however, uncertain by a factor of two.

It is interesting to note that by placing a magnet between the oven and the collision chamber, Lichten and Schultz could produce a beam of polarized atomic hydrogen. That is to say, the component of the spin of the bound electron along the imposed magnetic field lines would be either +1/2 or -1/2 according to the position of the oven. These polarized beams could then be used to measure, in terms of the total cross section, the probability of spin exchange occurring between the bound and the scattered electrons.

With a similar arrangement, Stebbings et al. (1960) used a Lyman-alpha detector to obtain the ratio of the 2s to the 2p excitation cross sections. They modulated the H(1s) beam from the oven at the rate of 100 cps by use of a toothed chopper wheel. This modulated signal allowed them to extend the range of their measurements out to 600 eV. The absolute values of $\sigma_{1s\rightarrow 2p}$ had been previously obtained by normalizing earlier (1s-2p) measurements to the Born approximation between 200 and 700 eV [Fite, Stebbings and Brackmann (1959)]. It is thought that this method of normalization is accurate in this energy range. The absolute value of $\sigma_{1s\rightarrow 2s}$ could thus be obtained in lower energy regions where the Born approximation is not valid. In reducing their data, however, Stebbings et al. (1960) assumed that in the presence of the quenching field that the excited hydrogen atoms radiated anisotropically. Because of this they multiplied their H(2s) measurements by two-thirds. But Lichten (1961) pointed out that the radiation was actually isotropic and hence the published values of Stebbings et al. should be increased by 50 percent.

The measured cross sections, above 12.1 eV, included not only the direct 1s-2s excitation cross section but also that contribution to the production of H(2s) due to cascade from higher levels excited from the ground state by electron impact. Using the transition probabilities given by Bethe and Salpeter (1957), Lichten and Schultz showed that the measured total 2s production cross section is equivalent to the sum of the direct 1s-2s cross section plus 21 percent of the 1s-3p excitation cross section. The 1s-3p curve was obtained by multiplying

$(\sigma_{1s\rightarrow 3p})_{Born}$ by the same energy dependent factor required to reduce $(\sigma_{1s\rightarrow 2p})_{Born}$ to the experimental curve obtained by Fite and Brackmann (1958) and Fite, Stebbings, and Brackmann (1959). The same general procedure was followed by both Lichten and Schultz, and Stebbings et al.

Finally a brief resume of the experimental results is in order. The deduced direct (1s-2s) excitation cross sections of Lichten and Schultz and of Stebbings et al. are shown in figure 6. Stebbings et al. claim an experimental accuracy of about ±10 percent near threshold but this soon drops to ±20 percent or more at higher energies. Lichten and Schultz claim an experimental accuracy at least two or three times that of Stebbings et al. for their metallic detector. However, their absolute cross sections, which are roughly twice those of Stebbings et al., depend on the normalization of their curve to the first Born approximation between 30 and 40 eV. Thus, although they seemed to have accurately determined the shape of the $\sigma_{1s\rightarrow 2s}$ curve, their experiment leaves the absolute value in doubt. Lichten and Schultz did make one absolute determination of $\sigma_{1s\rightarrow 2s}$ at 11.7 eV. The value obtained was $(.28 \pm .14)\pi a_o^2$, where a_o is the Bohr radius. This result is compatible with either the Born approximation normalization or the measurements of Stebbings et al. Hence the experimental results still leave the absolute value of the cross section in doubt by perhaps as much as a factor of two.

2. Early Theories

Previous to the Lichten and Schultz experiment in 1959, there had been a number of calculations of the excitation cross section $\sigma_{1s\rightarrow 2s}$. However, these were confined either to the first Born approximation, Bates and Miskelly (1957), or to the zeroth order (total angular momentum $L = 0$) partial wave – Erskine and Massey (1952), Massey and Moiseiwitsch (1953), Bransden and McKee (1956), and Marriott (1958). Much present evidence indicates that the results of the Born approximation are too high below 50 eV. Bates, Fundaminsky, Leech, and Massey (1950) pointed out the inadequacy of the Born approximation near the excitation threshold. Hummer and Seaton (1961) and others now doubt the accuracy of this approximation below 100 or 200 eV. Kingston, Moiseiwitsch and Skinner (1960) made a third order Born approximation calculation of $\sigma_{1s\rightarrow 2s}$. It is compatible with the corrected results of the experiment of Stebbings et al. (1960) at energies above 100 eV, but at lower energies the calculated values lie above the experimental curve of Stebbings et al. Although the authors take this as an indication of validity of the normalization procedures of Lichten and Schultz, they themselves claim no great accuracy for their calculation below 50 eV. All of the zero-order partial wave calculations fall far below the experimental results, over most of the experimental energy range. The obvious conclusion was that higher partial waves had to be taken into account.

Percival and Seaton (1957) published a study showing how the radial wave function for arbitrary angular momentum, L, could be included in the

(1s-2s-2p) close coupling approximation. After the experiment of Lichten and Schultz in 1959, a number of workers began to utilize this partial wave theory to develop close coupling computer programs which included the higher partial waves. The article by Burke and Smith (1962) in the Reviews of Modern Physics gives a good account of the work done up to that time. Subsequent papers by Burke, Schey and Smith (1963), Omidvar (1964), and Gailitis and Damburg (1963) should also be mentioned. Since at present the close coupling technique is the most popular one for low energy calculations, a brief description of it is included.

First let us delineate the exact problem and then investigate various approximate solutions. Consider an electron being scattered by a hydrogen atom which is originally in the 1s state. By neglecting the motion of the proton and taking its position as the origin of the coordinate system, the Schrödinger equation for the system can be written:

$$(H-E)\Psi(r_1\sigma_1, r_2\sigma_2) = 0 \qquad (1)$$

where $\underline{r}_1$ and $\underline{r}_2$ are the position vectors, respectively, of the free and of the bound electrons while σ_1 and σ_2 are the respective spin coordinates. Each of the spin coordinates may take the value 1/2 or -1/2, and the particles obey Fermi-Dirac statistics. For the transitions considered here, spin orbit interactions are negligible. Hence we may write

$$H-E = -\nabla_1^2 - \nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_{12}} - E \qquad (2)$$

In (2) H is the Hamiltonian and E is the total energy of the system, while r_{12} is the distance between the two electrons. All lengths are measured in Bohr radii, and energy in Rydbergs. Since the spin coordinates do not appear in the Hamiltonian, the spin and space dependent parts of the total wave function are separable and we can write

$$\Psi(\underline{r}_1\sigma_1, \underline{r}_2\sigma_2) = \chi(\sigma_1, \sigma_2)\,\Psi(\underline{r}_1, \underline{r}_2).$$

The problem thus concerns the interaction of two identical particles, obeying Fermi-Dirac statistics, in the field of an attractive center of force.[1, 2] By Fermi-Dirac statistics the total wave function must be antisymmetric under the exchange of coordinates; hence

$$\Psi(\underline{r}_1\sigma_1, \underline{r}_2\sigma_2) = -\Psi(\underline{r}_2\sigma_2, \underline{r}_1\sigma_1).$$

If $\chi(\sigma_1, \sigma_2)$ is symmetric, $\Psi(\underline{r}_1, \underline{r}_2)$ must be antisymmetric, and vice versa.

The spin wave function $\chi(\sigma_1, \sigma_2)$ may conveniently be assumed to be a common eigenfunction of the operators S_z and $\underline{S}^2$. Here S_z is the

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1 The scattering problem involving two identical particles is discussed in Mott, N. F., and Massey, H. S. W., The Theory of Atomic Collisions, 2nd Ed., Oxford, Clarendon Press, 1949, pages 102, 143.

2 The quantum mechanical theory of two identical particles is discussed at some length in Merzbacher, E., Quantum Mechanics, New York, John Wiley and Sons, Inc., 1961, Chapter 18.

z component and $\underline{S}^2$ is the square of the magnitude of the total spin operator. In units of $\hbar$ the eigenvalues of S_z are $M_S = \pm 1$ or 0, while the eigenvalues of $\underline{S}^2$ are $S = 1$ or 0. In terms of the one electron spin functions $\chi_1(\sigma_1)$ and $\chi_2(\sigma_2)$, the spin eigenfunctions of the two-particle system can be written in the form

$$\left.\begin{array}{lll} S=1 & M_S=1 & \chi_1(\tfrac{1}{2})\chi_2(\tfrac{1}{2}) \\ S=1 & M_S=0 & \frac{1}{\sqrt{2}}\left[\chi_1(\tfrac{1}{2})\chi_2(-\tfrac{1}{2})+\chi_1(-\tfrac{1}{2})\chi_2(\tfrac{1}{2})\right] \\ S=1 & M_S=-1 & \chi_1(-\tfrac{1}{2})\chi_2(-\tfrac{1}{2}) \end{array}\right\} \text{triplet}$$

$$S=0 \quad M_S=0 \quad \frac{1}{\sqrt{2}}\left[\chi_1(\tfrac{1}{2})\chi_2(-\tfrac{1}{2})-\chi_1(-\tfrac{1}{2})\chi_2(\tfrac{1}{2})\right] \quad \text{singlet}$$

The triplet spin functions are symmetric under the interchange of spin coordinates and therefore must multiply a space antisymmetric function. Similarly, the antisymmetric singlet spin function must multiply a space symmetric function. To obtain the probability of a given collision one must calculate the probability, using both symmetric and antisymmetric space functions, and then average over the spins. If the former probability is P_S (singlet) and the latter P_T (triplet), the total probability is

$$\frac{1}{4}\left[P_S + 3P_T\right] .$$

We may now proceed with the solution of the spatial problem and refer again to the spin only when calculating the total interaction probabilities.

The spacial wave function $\Psi(\underline{r}_1, \underline{r}_2)$ is a nonseparable function of its vector arguments, and since, therefore, the spacial problem cannot be solved exactly, some approximations must be made. A

reasonable approach is to expand $\Psi(\underline{r}_1, \underline{r}_2)$ in terms of the eigenfunctions of the total angular momentum, which commutes with H, and to write

$$\Psi(r_1, r_2) = \sum_{L=0}^{\infty} \Psi_L(r_1, r_2) \tag{3}$$

Since these eigenfunctions are orthogonal, substitution of Eq. (3) into Eq. (1) yields

$$(H-E)\Psi_L(\underline{r}_1, \underline{r}_2) = 0 \tag{4}$$

Up to this point no approximations have been made. If the $\Psi_L(\underline{r}_1, \underline{r}_2)$ could be found exactly and if all L were taken into account, then we would have the exact solution of the problem. Unfortunately the Ψ_L cannot be determined exactly.

The close coupling procedure is to expand $\Psi_L(\underline{r}_1, \underline{r}_2)$ in terms of the eigen states of the hydrogen atom. The coefficients of the expansion, which are functions of the position vector of the free electron, are found by numerical integration. If an infinite number of terms were included in the expansion, the solution of the problem would be exact. Omidvar (1964) has given the explicit form of the expansion as:

$$\Psi_L(\underline{r}_1, \underline{r}_2) = (1+\beta P_{12}) \sum_{n_2 l_2 l_1} \sum_{m_2 m_1} C^{l_2 l_1 L}_{m_2 m_1 M} \varphi(n_2 l_2 m_2, \underline{r}_2) \times r_1^{-1} U(k_{n_2} l_1, r_1) Y_{l_1 m_1}(\Omega_1) \tag{5}$$

where

$$\varphi(n_2 l_2 m_2) = r_2^{-1} R(n_2 l_2, r_2) Y_{l_2 m_2}(\Omega_2) \tag{6}$$

is the hydrogen atom wave function with radial part $r_2^{-1}R(n_2\, \ell_2,\, r_2)$ and angular part $Y_{\ell_2 m_2}(\Omega_2)$ and quantum numbers $n_2\ \ell_2\ m_2$; $r_1^{-1}U(k_{n_2}\, \ell_1,\, r_1)$ is the radial part and $Y_{\ell_1 m_1}(\Omega_1)$ is the angular part of the free electron wave function with quantum numbers $k_{n_2}\ \ell_1\ m_1$. The relationship between the wave number k_{n_2} and n_2 is given by

$$k_{n_2}^2 = \left(E + n_2^{-2}\right) \tag{7}$$

The constants $C^{\ell_2\ \ell_1\ L}_{m_2\ m_1\ M} = (\ell_1\ \ell_2\ m_1\ m_2 \mid LM)$ are the necessary vector coupling (Clebsch Gordon) coefficients which make the expansion (5) an eigenfunction of the total angular momentum L. To insure that the total wave function is either symmetric (antiparallel spins) or antisymmetric (parallel spins), it is multiplied by the coefficient $(1 + \beta P_{12})$. The operator P_{12} interchanges $\underline{r}_1$ and $\underline{r}_2$ while β is +1 in the symmetric and -1 in the antisymmetric case.

An example is the L = 0, (1s-2s) wave function used by Marriott (1958):

$$\psi_0(1s\text{-}2s) = (1+\beta P_{12})\, r_1^{-1} \left\{ U(k_1, 0, r_1)\, \varphi(100, r_2) + U(k_2, 0, r_1)\, \varphi(200, r_2) \right\} \tag{8}$$

The free electron radial wave functions are required to vanish at $r_1 = 0$ and to have the asymptotic forms

$$\left.\begin{aligned} \lim_{r\to\infty} U(k_1,0,r) &= k_1^{-1}\sin k_1 r + a e^{ik_1 r} \\ \lim_{r\to\infty} U(k_1,0,r) &= b\, e^{ik_1 r} \end{aligned}\right\} \qquad (9):$$

Calculations which assume that only the 1s and 2s channels are open are called (1s-2s) CC calculations; those which have the 1s, 2s and 2p channels open are called (1s-2s-2p) CC calculations.

In order that the close coupling $\Psi_L(\underline{r}_1, \underline{r}_2)$ should closely approximate the exact wave function, the expectation value of the energy operator is minimized with respect to the radial parts of the free electron wave functions:

$$\delta \int \Psi_L^*(\underline{r}_1,\underline{r}_2)[H-E]\Psi_L(\underline{r}_1,\underline{r}_2)\, d^3\underline{r}_1\, d^3\underline{r}_2 = 0 \qquad (10)$$

It has been shown by Kohn (1948) that the differences between the scattering amplitudes obtained from these equations and the exact scattering amplitudes are quadratic in the difference between $\Psi_L(\underline{r}_1, \underline{r}_2)$ and the exact wave function.

Equation (10) is equivalent to a coupled set of integral differential equations which must be solved in order to obtain the free electron radial wave functions $U(k_{n_2}\ \ell_1, r_1)$. It is customary nowadays to solve these equations numerically. In practical calculations it is impossible to solve Eq. (4) explicitly since only a finite number of terms can be included in the expansion. If a truncated expansion is used, then the CC Ψ_{trunc} is not a solution

of the Schrödinger Eq. (4).[3]

Omidvar (1964), using the (1s-2s-2p) CC expansion, took into account all partial waves from $L = 0$ to ∞. Close coupling procedures were used for the low numbered partial waves, while the effect of the higher partial waves was estimated using the regular Born approximation. The CC calculations were broken off at the value of L for which the CC and the regular partial wave Born approximation were in substantial agreement. His results agree very closely with the earlier (1s-2s-2p) CC calculation by Burke, Schey and Smith (1963).

The (1s-2s) CC and (1s-2s-2p) CC total cross sections $\sigma_{1s\rightarrow 2s}$ are shown in Figure 6. As can be seen, they would tend to confirm the normalization procedure used by Lichten and Schultz in reducing their experimental data, even though near threshold they differ substantially from the experimental curve of Lichten and Schultz. One may still legitimately wonder, however, just how accurate even the (1s-2s-2p) CC calculation is. One test would be to include more terms in the close coupling expansion of the $\psi_i(\underline{r}_1, \underline{r}_2)$. Greater confidence would be attained, however, if there were an accurate alternate method to the CC procedure. In the next chapter such a method is outlined, and a calculation is carried out which calls in question the accuracy of the (1s-2s) CC calculation and therefore, by inference, also the (1s-2s-2p) CC calculation.

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[3] Mott, N. F. and Massey, H. S. W., op. cit., pages 141, 217, 260.

CHAPTER II

The Nonadiabatic Theory

1. Introduction

The nonadiabatic theory for atomic scattering is an extension of a method suggested by Breit, and first used by Luke, Meyerott and Clendenin (1952) for calculating the energy of some excited states of 2-electron atoms and ions. The first papers on the nonadiabatic scattering theory by Temkin (1960, 1961, 1962A) dealt with the problem of the elastic scattering of an S-wave electron by a hydrogen atom in its ground state. At this time there was renewed interest in this problem because Rosenburg, Spruch and O'Malley (1960) had just calculated rigorous upper bounds, $a_s < 6.23$, and $a_t < 1.92$, for the singlet and triplet scattering lengths in the scattering of electrons from atomic hydrogen. They assumed that the H^- ion has only one bound state, with singlet spin. These scattering lengths, which are equivalent to the zero energy scattering cross sections, were 15 percent below the results of the most elaborate calculations performed up to that time. For references to these earlier works see Bransden, Dalgarno, John and Seaton (1958).

The nonadiabatic theory proved a very powerful tool in attacking this problem and in calculating the elastic phase shifts below 10.2 eV, the (1s-2s) excitation threshold. For the singlet scattering length Temkin (1962A) obtained $a_s = 5.6$, and in the triplet case Temkin and

Sullivan (1963) obtained $a_t = 1.7683$. To date this is one of the two most accurate sets of calculations of the S-wave elastic phase shifts below 10.2 eV. The other calculation of comparable accuracy is that of Schwartz (1961) who used Kohn's variational principle and 50 trial functions of the Hylleraas type. Schwartz obtained the values $a_t = 1.7686 \pm .0002$ and $a_s = 5.965 \pm .003$.

The nonadiabatic theory has since been applied, among other problems, to positron-hydrogen scattering, Temkin (1962B), and to the problem of one electron molecules, particularly $(H_2)^+$, Temkin (1963A).

2. Inelastic S-wave Scattering[1]

The radial and angular parts of the exact angular momentum eigenfunctions are separable.[2] The angular part is a function of the Eulerian angles Θ, Φ, and Ψ, while the radial part depends on the three scalar quantities r_1, r_2, and θ_{12}. As in Chapter I, $\underline{r}_1$ and $\underline{r}_2$ are, respectively, the radius vectors from the proton to the free and to the bound electron, while θ_{12} is the angle between $\underline{r}_1$ and $\underline{r}_2$. The orientation of the $(\underline{r}_1, \underline{r}_2)$ plane is described by Θ, Φ, and Ψ. We are particularly interested here in the zero angular momentum wave function. In this case the angular part is a

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1 The discussion in the following two sections is essentially taken from Temkin (1962A), but modified so as to include inelastic processes.

2 Morse, P. M., and Feshbach, H., Methods of Theoretical Physics, Vol. II, New York, McGraw-Hill (1953), p. 1719.

constant independent of ϖ, Φ, and Ψ. Hence we can write

$$\Psi_0(r_1, r_2) = \Psi(r_1, r_2, \theta_{12}), \tag{11}$$

and the Schrödinger equation takes the form

$$\left\{-\frac{1}{r_1}\frac{\partial^2}{\partial r_1^2} - \frac{1}{r_2}\frac{\partial^2}{\partial r_2^2} - \left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\left(\sin\theta_{12}\frac{\partial}{\partial\theta_{12}}\right)\right. \tag{12}$$

$$\left. -\frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_{12}} - E\right\}\Psi(r_1, r_2, \theta_{12}) = 0 .$$

If we take advantage of the fact that

$$\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\left[\sin\theta_{12}\frac{\partial}{\partial\theta_{12}}P_l(\cos\theta_{12})\right] = -l(l+1)P_l(\cos\theta_{12}), \tag{13}$$

the wave function may be expanded in terms of the Legendre polynomials, $P_l(\cos\theta_{12})$:

$$\Psi(r_1, r_2, \theta_{12}) = \frac{1}{r_1 r_2}\sum(2l+1)^{1/2}\Phi_l(r_1 r_2)P_l(\cos\theta_{12}) . \tag{14}$$

Substitution of (14) into (12) gives an infinite set of coupled equations:

$$\left\{\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} - l(l+1)\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right) + E + \frac{2}{r_1} + \frac{2}{r_2} - M_{ll}\right\}\Phi_l(r_1 r_2) \tag{15}$$

$$= \sum_{m=0}^{\infty}{}' M_{lm}\Phi_m(r_1 r_2) .$$

The prime on the right hand side sum means that the term $m = l$ is to be omitted. In the region $r_1 > r_2$

$$M_{lm} = (2l+1)^{1/2}(2m+1)^{1/2}\sum_{n=0}^{l+m}\frac{r_2^n}{r_1^{n+1}}$$

$$\times\int_0^{\infty}P_l(\cos\theta)P_m(\cos\theta)P_n(\cos\theta)\sin\theta\,d\theta .$$

Under exchange $\underline{r}_1 \rightleftarrows \underline{r}_2$, the three coordinates of the S-wave problem transform according to $r_1 \rightleftarrows r_2$, and $\theta_{12} \rightleftarrows \theta_{12}$. Hence the required symmetry conditions are that

$$\psi(r_1, r_2, \theta_{12}) = \pm \psi(r_2, r_1, \theta_{12}).$$

In terms of the expansion Φ_ℓ this implies (as a necessary and sufficient condition) that

$$\Phi_\ell(r_1\ r_2) = \pm \Phi_\ell(r_2\ r_1). \tag{16}$$

Equation (16) can be satisfied, and at the same time the problem can be restricted to the region $r_1 > r_2$ by imposing the additional boundary condition

$$\begin{aligned} \Phi_\ell(r_1\ r_2)\Big|_{r_1 = r_2} &= 0 \qquad \text{triplet} \\ \frac{\partial}{\partial n}\Phi_\ell(r_1\ r_2)\Big|_{r_1 = r_2} &= 0 \qquad \text{singlet}. \end{aligned} \tag{17}$$

With this boundary condition the solution of the problem in the half plane $(r_1 > r_2)$ is identical to the solution in the other half plane $(r_1 < r_2)$, except for a minus sign in the singlet case. In Eq. (17) $\partial/\partial n|_{r_1=r_2}$ is the derivative normal to the line $r_1 = r_2$; specifically

$$\frac{\partial}{\partial n}\Big|_{r_1=r_2} \propto -\frac{\partial}{\partial r_1} + \frac{\partial}{\partial r_2}.$$

Because of the $(r_1 r_2)^{-1}$ factor in Eq. (14), we have in both cases

$$\Phi_\ell(r, 0) = 0. \tag{18}$$

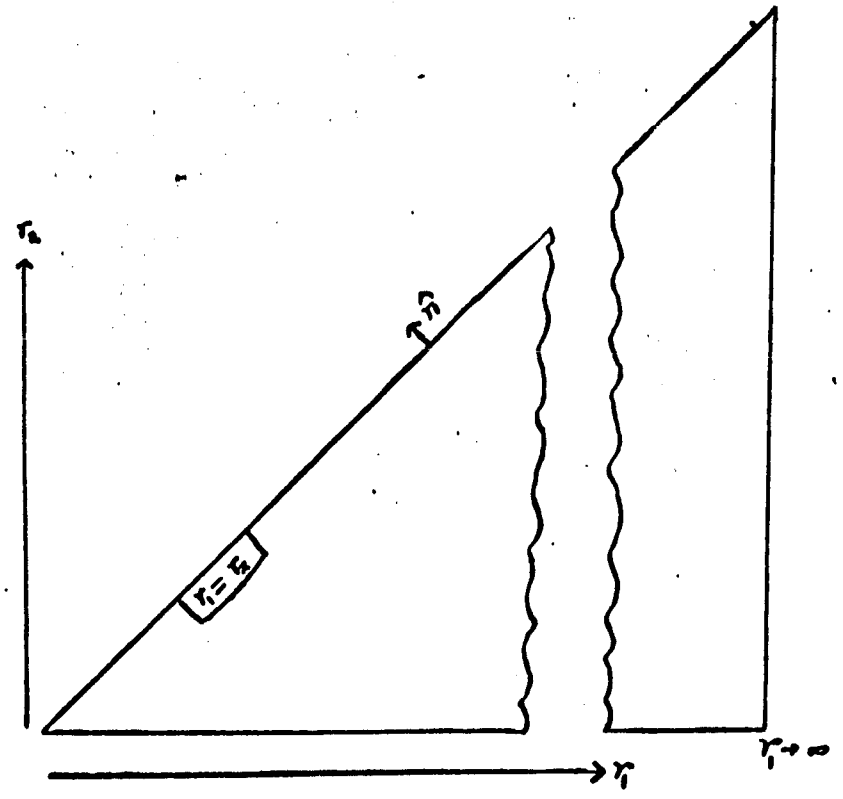

Figure 1. The $r_1 > r_2$ triangle, to which the whole mathematical problem is restricted. $\hat{n}$ is the outward unit normal to the boundary of the triangle.

For energies between 10.2 and 12.09 eV the asymptotic conditions on the $\Phi_{L_f}(r_1 r_2)$ are

$$\left.\begin{aligned} &\lim_{r_1\to\infty} \Phi_0(r_1 r_2) = \left(\frac{A}{k_1}\sin k_1 r_1 + a e^{i k_1 r_1}\right) R_{1s}(r_2) + b e^{i k_2 r_1} R_{2s}(r_2) \\ &\lim_{r_1\to\infty} \Phi_1(r_1 r_2) = d e^{i k_2 r_1} R_{2p}(r_2) \\ &\lim_{r_1\to\infty} \Phi_{L_f}(r_1 r_2) = 0 \quad , \; l > 1 \; . \end{aligned}\right\} \qquad (19)$$

In (19) A is the arbitrary normalization of the incident plane wave while the parameters a, b, and d describe, respectively, the scattering amplitudes for the processes 1s-1s, 1s-2s, 1s-2p. The quantities k_n are defined in Eq. (7), and, as previously stated, the $r^{-1}R_{ns}(r)$ are hydrogenic radial wave functions.

As the incident electron energy is raised above 12.09 eV, other channels corresponding to the bound states of hydrogen become open. For energies above 13.6 eV a dense infinity of ionization states is also accessible. Since it is clearly impossible to treat all these cases, it will be assumed, in what follows, that all channels are closed except those specifically stated to be open.

The S-wave scattering cross sections $\sigma_{1s\to 1s}$ and $\sigma_{1s\to 2s}$ are completely specified, for $10.2 < k_1^2 < 12.09$ eV, by the coupled set of Eqs. (15) subject to the boundary conditions (17), (18) and (19). Clearly one must solve such a set of equations in some approximate manner. One possible procedure is to define a zeroth order approximation, Temkin (1962A), and then use this either in a multipole expansion analogous to Temkin's method, or perhaps alternatively in an iteration scheme utilizing the two dimensional integration procedures developed by Temkin and Sullivan (1963). Both the multipole expansion and the iterative scheme have been tentatively examined and both have been found to be much more difficult than in the case of elastic scattering. Therefore, in this thesis only the solution of the zeroth order approximation is presented.

3. The Zeroth order Approximation

The zeroth order approximation is defined as follows. Note that

$$M_{0m} = \frac{2}{(2m+1)^{1/2}} \frac{r_<^m}{r_>^{m+1}} \tag{20}$$

hence the explicit form of the $\Phi_0(r_1 r_2)$ equation is

$$\left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2} + E\right)\Phi_0(r_1 r_2) = \sum_{m=1}^{\infty} \frac{2}{(2m+1)^{1/2}} \frac{r_<^m}{r_>^{m+1}} \Phi_m(r_1 r_2). \tag{21}$$

Let us approximate this equation by neglecting the right hand side. The zeroth order wave function $\Phi_0^{(0)}(r_1 r_2)$ is then defined by

$$\left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2} + E\right)\Phi_0^{(0)}(r_1 r_2) = 0, \tag{22}$$

subject to the boundary conditions (17), (18), and the asymptotic condition

$$\lim_{r_1 \to \infty} \Phi_0^{(0)}(r_1 r_2) = \left(\frac{A}{k_1}\sin k_1 r_1 + a_0 e^{ik_1 r_1}\right) R_{1S}(r_2) \tag{23}$$
$$b_0 e^{ik_2 r_1} R_{2S}(r_2) .$$

The zeroth order equation (22) is of particular interest because Temkin (1962A) has shown that the exchange approximation, which uses a trial ψ_{EA} not depending on the angle θ_{12}, cf. Eq. (8)

$$r_1 r_2 \psi_{EA} = (1 + \beta P_{12})(U_1(r_1) R_{1S}(r_2) + U_2(r_1) R_{2S}(r_2)), \tag{8}$$

for the S-wave function, is in fact a variational solution of only that part of the original Schrödinger equation corresponding to (22). Consider the variational solution of the complete S-wave problem, Eq. (12), with any (symmetric or antisymmetric) function $f(r_1, r_2)$--

Ψ_{EA} from Eq. (8) for instance. We have then

$$\delta_u \int f^*(r_1,r_2)(H-E)f(r_1,r_2)\,d^3r_1\,d^3r_2 = 0 \qquad (24)$$

Here (H-E) represents the operator in the curly brackets in Eq. (12). The term $\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\left(\sin\theta_{12}\frac{\partial}{\partial\theta_{12}}\right)$ in (24) will vanish since $f(r_1,r_2)$ is independent of θ_{12}. Next consider the matrix element of the complete interaction, $+2/r_1+2/r_2-2/r_{12}$, in (24):

$$\iint f^*(r_1,r_2)\left(\frac{2}{r_1}+\frac{2}{r_2}-\frac{2}{r_{12}}\right)f(r_1,r_2)\,d^3r_1\,d^3r_2$$

$$\propto \int_0^\infty\int_0^\infty |r_1 r_2 f(r_1,r_2)|^2\,\frac{2}{r_<}\,dr_1\,dr_2$$

$$= 2\int_0^\infty dr_1\int_0^{r_1} dr_2\,|r_1 r_2 f(r_1 r_2)|^2\,\frac{2}{r_2}\ .$$

In these equations $r_<$ is the lesser and $r_>$ the greater of (r_1,r_2). The (anti) symmetry of $f(r_1,r_2)$ is used in the derivation as well as the fact that

$$\int_0^\pi \frac{1}{r_{12}}\sin\theta_{12}\,d\theta_{12} = \int_0^\pi \frac{\sin\theta_{12}\,d\theta_{12}}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_{12}}}$$

$$= \frac{2}{r_>}\ .$$

Hence the effective Hamiltonian in Eq. (24) is of the form

$$H_0 = -\frac{\partial^2}{\partial r_1^2} - \frac{\partial^2}{\partial r_2^2} - \frac{2}{r_<}$$

which is, of course, the form of the Hamiltonian in Eq. (22).

The zero angular momentum portion of the (1s-2s) close coupling approximation, Marriott (1958), has a wave function similar to Eq.(8) and therefore Marriott obtained a solution of Eq. (22). Thus the

solution of the zeroth order equation obtained in this thesis will serve as an immediate check on the close cou ing procedure, as well as serving as the basis of later, more exact, calculations of the $L = 0$ portion of the cross sections $\sigma_{1s\to 1s}$ and $\sigma_{1s\to 2s}$. The difference between the zeroth order problem and the (1s-2s) CC problem lies in the methods of solution that were used. This is discussed further in the next section.

4. Solution of the Zeroth Order Problem

In summary the zeroth order problem consists of the equation

$$\left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2} + E\right) \Phi_0^{(0)}(r_1 r_2) = 0 \tag{22}$$

and the boundary conditions

$$\Phi_0^{(0)}(r_1, 0) = 0 \tag{18}$$

$$\lim_{r_1\to\infty} \Phi_0^{(0)}(r_1 r_2) = \left(\frac{A}{k_1}\sin k_1 r_1 + a_0 e^{ik_1 r_1}\right) R_{1s}(r_2) + b_0 e^{ik_2 r_1} R_{2s}(r_2) \tag{23}$$

and

$$\left.\begin{aligned} \Phi_0^{(0)}(r_1 r_2)\big|_{r_1 = r_2} &= 0 \qquad \text{Triplet} \\ \frac{\partial}{\partial n}\Phi_0^{(0)}(r_1 r_2)\big|_{r_1 = r_2} &= 0 \qquad \text{Singlet} \end{aligned}\right\} \tag{25}$$

In the remainder of the thesis the subscripts on a_0 and b_0 will be omitted. Equation (22) can describe only relative s-states and is therefore also called the "relative-s problem". While it does possess separable solutions, the imposed boundary conditions make

$\Phi_o^{(o)}(r_1 r_2)$ non-separable. Following Temkin (1962A), $\Phi_o^{(o)}(r_1 r_2)$ will be expanded in terms of the separable eigenfunctions of Eq. (22):

$$\Phi_o^{(o)}(r_1 r_2) = \left(\frac{A}{k_1}\sin k_1 r_1 + a e^{ik_1 r_1}\right) R_{1s}(r_2) + b e^{ik_2 r_1} R_{2s}(r_2) + \left(\sum_n + \int dp\right) C_n e^{-\chi_n r_1} R_{ns}(r_2) \quad , n \geq 3 . \tag{26}$$

The sum plus integral means, as usual, that the continuum s-states of hydrogen in addition to the discrete states must be included. All the terms in this sum plus integral go exponentially to zero with large r_1, and they are therefore often called virtually excited states. For the discrete states

$$\chi_n = (1 - n^{-2} - k_1^2)^{1/2} , \tag{27}$$

and for the continuum

$$\chi_p = (1 + p^2 - k_1^2) \quad . \tag{28}$$

With this relationship each term of (26) is an exact solution of (22).

The expansion (26) automatically satisfies two of the boundary conditions (23) and (18), but not the third (25). In order to satisfy (25), at least approximately, we determine a, b, and C_n by the variational conditions given in Temkin (1962A):

$$\frac{\partial I_S}{\partial \chi_j} = 0 \qquad \chi_j = a, \arg(b), C_n \quad n = 3, \ldots, N+2 . \qquad \frac{\partial I_T}{\partial \chi_j} = 0 \tag{29}$$

N is the number of terms, beyond the first two, included in the expansion (26), and the diagonal integrals I_T and I_S are

$$I_T = \int_0^\infty |\Phi_0^{(0)}(r_1 r_2)|^2_{r_1=r_2} dr$$

$$I_S = \int_0^\infty |\frac{\partial}{\partial n} \Phi_0^{(0)}(r_1 r_2)|^2_{r_1=r_2} dr \qquad (30)$$

Since a and the (C_n) are complex, $2N+3$ real equations result from (29). These equations are linear in the C_n; hence 2N of them may be solved immediately to obtain the (C_n) in terms of Re(a), Im(a), and Arg(b). The procedure followed is analogous to that outlined in part four of Temkin (1962A). The solution for the triplet case is given in Appendix A. The integrals in Eq. (30) were obtained in analytic form (see Appendix B), and were checked by numerical integration. However, in the singlet case, due to the difficulty of the numerical integrations, the analytic results were in some cases only checked to one or two significant figures. In order to obtain sufficient accuracy it was necessary to solve for the C_n using double precision arithmetic, i.e., 16 significant figures were retained in the calculations. The remaining three equations are highly nonlinear in Re(a), Im(a), and Arg(b), and were therefore solved numerically. All calculations were performed on the IBM 7094 computer of the Theoretical Division of the Goddard Space Flight Center.

"It is worth pointing out the converse nature of this technique of solution to those usually employed. In most cases one approximates the exact solution in terms of functions which are not solutions of the equation, but do satisfy all the boundary conditions. In close-coupling, for example, the basis functions are solutions of part but

not all of the equations. The method that is here presented utilizes functions which are complete solutions of the equation but do not satisfy all the boundary conditions. In the latter method the smallness of the deviation from the boundary condition is a very reliable index of the quality of the solution (providing this difference is small enough)." [3]

The scattering cross sections obtained from (23) are:

$$\sigma_{1S\to 1S} = 4\pi \frac{|a|^2}{|A|^2} \tag{31}$$

$$\sigma_{1S\to 2S} = \frac{4\pi k_2}{k_1} \frac{|b|^2}{|A|^2} \tag{32}$$

In order to insure conservation of current, the constants A, a, and b are required to obey the relationship

$$\mathrm{Im}\,(A^{*}\, a) = k_1 |a|^2 + k_2 |b|^2 \quad . \tag{33}$$

To facilitate the solution of certain non-linear equations which appear in the problem, let

Case (i) $\quad A = k_1(1-ia),$

and (34)

$$a = x + iz^2$$

$$b = (k_1/k_2)^{1/2}\, z e^{i\delta} \quad .$$

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[3] Temkin (1962A), section iv.

As a check on the calculations the singlet case was also solved with[4]

Case (ii) $A = k_1$,

and

$$a = (xe^{2i\delta_1} - 1)/2i \qquad (35)$$

$$b = \tfrac{1}{2}\left[(k_1/k_2)(1-x^2)\right]^{1/2} e^{i(\delta_1+\delta_a)} .$$

In both cases the form of b is so chosen that Eq. (33) was automatically satisfied. Hence the complex numbers a and b are fully determined by the real numbers Re(a), Im(a), and Arg(b). The results of the computation are presented in Sec. 8 of this chapter.

5. The Scattering Matrix

If an exact solution were obtained for the zeroth order problem, then the reciprocity condition[5] should be fulfilled and the scattering cross sections σ_{2s-2s} and σ_{2s-1s} could also be obtained from this same calculation. Although we have no direct check on how closely the reciprocity condition is fulfilled, it is expected that when I_S and I_T are small enough, reciprocity is satisfied to a good degree of approximation. The cross section σ_{2s-1s} follows immediately from the

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4 Case (i) was suggested by Massey and Moiseiwitsch (1953), while case (ii) was taken from Karplus and Rodberg (1959). The difference between case (i) and case (ii) should be merely computational. However, as indicated in Appendix A, the equations to be solved in the two cases are quite different. Hence, if the symmetry boundary condition, Eq. (17), is not satisfied sufficiently well, the two cases may give quite different answers.

5 A derivation of the reciprocity theorem as it applies to scattering matrices is given by Blatt, J. M., and Weisskopf, V. F., Theoretical Nuclear Physics, New York, John Wiley and Sons (1952), p. 528.

reciprocity condition; one form of which is

$$\sigma_{2s\text{-}1s} = (k_1/k_2)^2 \, \sigma_{1s\text{-}2s}$$

It is, however, necessary to introduce the scattering matrix S in order to obtain $\sigma_{2s\text{-}2s}$.

Many forms of the asymptotic boundary condition, Eq. (23), have been introduced by various authors. Two of the more common variations are of the following types:

$$\lim_{r_1\to\infty} \Phi_0^{(0)}(r_1 r_2) = (\sin k_1 r_1 + T_{11} e^{ik_1 r_1}) R_{1s}(r_2) + (k_2/k_1)^{1/2} T_{12} e^{ik_2 r_1} R_{2s}(r_2) \tag{36}$$

$$\lim_{r_1\to\infty} \Phi_0^{(0)}(r_1 r_2) = (e^{-ik_1 r_1} - S_{11} e^{ik_1 r_1}) R_{1s}(r_2) - (k_2/k_1)^{1/2} S_{12} e^{ik_2 r_1} R_{2s}(r_2) \tag{37}$$

In Eq. (36) the T_{ij} are elements of the transmission matrix T while in Eq. (37) the S_{ij} are the elements of the scattering matrix S. The coefficient $(k_2/k_1)^{1/2}$ multiplying T_{12} and S_{12} is introduced so that T_{ij} and S_{ij} will be symmetric.

Equations (23) and (36) are related in the following way:

$$T_{11} = k_1 a A^* / |A|^2 \tag{38}$$

$$T_{12} = k_1 (k_1/k_2)^{1/2} b A^* / |A|^2 . \tag{39}$$

The S and T matrices defined by Eqs. (36) and (37) are related by

$$S = 1 + 2iT \tag{40}$$

Here 1 is the unit matrix.

If the S matrix is required to conserve probability current, then it will be unitary:

$$SS^{\dagger} = 1. \tag{41}$$

If the reciprocity condition also holds, then the S matrix will be symmetric:

$$S_{12} = S_{21} . \tag{42}$$

From Eq. (41) S_{22} may be found to be

$$S_{22} = \frac{-S_{11}^{*} S_{12} S_{21}}{|S_{12}|^2} . \tag{43}$$

Finally, the reaction cross sections are given by the formula

$$\sigma_{is \rightarrow js} = \pi |\delta_{ij} - S_{ij}|^2 / k_1^2 , \tag{44}$$

where δ_{ij} is the Kronecker delta function. The σ_{2s-2s} thus obtained are listed in Table VI.

6. Internal Consistency of the Solution

The diagonal integrals I_S and I_T, Eq. (30), should ideally be zero. Presumably if enough terms could be taken in the wave function expansion, Eq. (26), this should occur to an arbitrary precision, however, for $N > 8$ the determinant of the C_j $(j = 1, N)$ was generally too small for accurate results to be obtained. By trial and error, sets of terms in the expansion were chosen which minimized I_S and I_T. The confidence we have in our results depends both on the smallness of I_S and I_T and on the consistency of the cross sections obtained by choosing different sets of virtual eigenstates. The magnitudes of the

obtainable I_S and I_T are shown in Table I. As can be seen, I_S and I_T are both quite small for energies less than that required to excite the 3s level of hydrogen. As soon as the 3s threshold is passed, there is a marked increase in the size of the diagonal integrals (particularly in the singlet case). The size of the diagonal integral continues to increase out to 30.6 eV. At these higher energies there is also a marked decrease in the agreement of the cross sections obtained by choosing different sets of virtual continuum states. Again this was most bothersome in the singlet case.

Table I

Satisfaction of the diagonal boundary condition, $I_S = I_T = 0$, at various incident momenta k_1.

k_1 (atomic units)	I_S	I_T
0.8662	1×10^{-5}	3×10^{-5}
0.9	3×10^{-6}	2×10^{-5}
0.94	2×10^{-5}	3×10^{-5}
	3s threshold	
0.95	1×10^{-3}	1×10^{-4}
1.0	5×10^{-3}	1×10^{-3}
1.1	2×10^{-2}	2×10^{-3}
1.2	4×10^{-2}	4×10^{-3}
1.5	1×10^{-1}	1×10^{-2}

Table II

Investigation of the internal consistency of the singlet nonadiabatic calculations. The scattering cross sections are given in units of πa_o^2 with the statistical factor 1/4 included. Each solution is specified by the virtual states included in the expansion (26). The discrete states are defined by their principle quantum numbers 'n', while the continuum states are defined by their momentum 'p'. The case (i) results are given on the first line of each row while the case (ii) results are in parentheses beneath them.

k_1 atomic units	I_S	1s-2s	1s-1s	virtual states: discrete n	virtual states: continuum p
0.9	3×10^{-6}	0.0339	0.4674	3,4	0.05,0.3,0.6,0.9,1.1
	(1×10^{-6})	(0.0338)	(0.4674)		
0.9	1×10^{-5}	0.0339	0.4674	3	0.05,0.3,0.5,0.7,0.9 1.1
	(7×10^{-6})	(0.0339)	(0.4674)		
0.9	1×10^{-4}	0.0334	0.4676	4	0.05,0.3,0.5,0.7,0.9 1.1
	(5×10^{-5})	(0.0335)	(0.4676)		
0.9	5×10^{-4}	0.0309	0.4680	-	0.05,0.3,0.5,0.7,0.9 1.1,1.3
	(3×10^{-4})	(0.0310)	(0.4684)		
0.9	8×10^{-4}	0.0289	0.4672	-	0.2,0.4,0.6,0.75,0.9 1.05
	(7×10^{-4})	(0.0291)	(0.4680)		
1.0	5×10^{-3}	0.0469	0.3263	-	0.05,0.25,0.45,0.65, 0.85,1.0,1.15,1.30
	(3×10^{-3})	(0.0488)	(0.3290)		
1.0	7×10^{-3}	0.0463	0.3283	-	0.05,0.3,0.6,0.8,1.0 1.2,1.4,1.6
	(4×10^{-3})	(0.0481)	(0.3319)		
1.5	1×10^{-1}	0.0131	0.0958	-	1.15,1.23,1.33,1.43, 1.53,1.63
	(8×10^{-2})	(0.0196)	(0.1126)		

For the singlet case this behavior is illustrated in Table II by the two top entries for $k_1 = 0.9$ and the entries for $k_1 = 1.0$ and $k_1 = 1.5$. These entries represent some of the better runs obtained at these energies. The uncertainty in the singlet results can be gauged by comparing case (i) and case (ii) results. At the higher energies the triplet results seem to be quite a bit more accurate than the singlet results.

Above the 3s threshold, Tables I and II indicate that the symmetry boundary condition, Eq. (25), has not been adequately fulfilled. Part of the difficulty may lie in the restricted asymptotic boundary condition, Eq. (23), for in reality the 3s and higher energy channels should be included at some of the incident energies we consider. However, it is our opinion that the chief difficulty above the 3s threshold is not the absence of, for example, the 3s state from the asymptotic region, but lies rather in its absence from the region of interaction. Partial confirmation of this can be found in the last four $k_1 = 0.9$ entries in Table II which illustrate the effect of omitting various low energy virtual states from the expansion. Experience has indicated, however, that a prudent choice of continuum states at energies above 12.1 eV will minimize the difficulties caused by the incompleteness in the expansion, Eq. (26).

A more relevant question is how these cross sections will change by virtue of the redistribution of current when the totality of open channels is included. Clearly the present calculation cannot answer that question, although in some sense the assumption must be made that

their effect is small. For if it were not, then the calculation of scattering in the ionization region would a complete impossibility, because their inclusion would entail a wave function containing not only a discrete infinity of bound excited states but a dense infinity of ionized states as well. It is our opinion that in close coupling, for example, when additional states are added at an energy where they may be excited, their main effect arises from the increased flexibility they allow the wave function in the region of interaction rather than in the opening of the channels that they afford. Thus the present method, which places virtually no restriction on the number of terms that can describe the wave function in the region of interaction, is expected to contain most of the effects on the 1s and 2s channels of a close coupling expansion with a similar number of terms.

7. Effective Range Expansion About the 2s Threshold

A final check was made to insure that our calculation was compatible with previous nonadiabatic (NA) calculations below the 2s threshold. Ross and Shaw (1961) have recently developed a multichannel effective range theory. This is an extension of the ordinary (single channel) effective range theory which can in principle describe all channels of a reaction both above and below the threshold for a new channel. The correlation is accomplished in terms of a real symmetric M matrix whose elements around threshold may be expanded in a power series in the energy. The first two of these coefficients reduce essentially to the scattering length and effective range in the

one channel case. The M matrix has been used by Damburg and Peterkop (1962) to extrapolate the results of 1s-2s close coupling calculations immediately above the 2s threshold to infer the elastic scattering below threshold. In the same spirit we have extrapolated our present NA results to below threshold. In this case, however, the extrapolation was in the nature of a check as the NA results below threshold have already been calculated.[6] For compatibility the extrapolated values of σ_{1s-1s} should then closely match the computed zeroth order NA σ_{1s-1s} below threshold. The usefulness of this check was brought home in our present calculations, when the values which had been computed at an earlier stage gave an extrapolated singlet $_{1s-1s}$ that was not compatible with the explicitly calculated values below threshold. This led to the discovery of a machine programming error which had caused earlier singlet results to indicate a spuriously high peak in σ_{1s-2s} cross section just above the 2s threshold, cf. Kyle and Temkin (to be published).

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6 A. Temkin and R. Pohle, Phys. Rev. Lett. 10, 22 (1963). It should be emphasized that only results of the zeroth order or relative s-wave problem of this reference are being considered and these show only one resonance. On the other hand, the inclusion of higher relative partial waves introduced more resonances. Cf. the erratum to the above, Phys. Rev. Lett. 10, 268 (1963); A. Temkin, NASA Tech. Note D-1720; A. Temkin, Proceedings of the Third International Conference on the Physics of Electronic and Atomic Collisions (Amsterdam, North-Holland Publishing Co., to be published); and Gailitis and Damburg, Proc. Phys. Soc. 82, 192 (1963).

The T and M matrices are related for relative s-wave scattering by the equation[7]

$$T = k^{1/2}(M - ik)\,k^{1/2} \tag{45}$$

In this equation k is considered to be a diagonal matrix with diagonal elements k_i. The elastic scattering is then given by

$$\sigma_{1s\text{-}1s} = 4\pi(M_{22}^2 + k_2^2)/\left|(M_{11}-ik_1)(M_{22}-ik_2)-M_{12}M_{21}\right|^2 \tag{46}$$

Expanding the elements of M_{ij} about a reference incident electron energy E_o, we obtain

$$M_{ij}(E) = M_{ij}(E_o) + \tfrac{1}{2}R_{ij}(E-E_o) + \quad \ldots \tag{47}$$

In the effective range approximation the series is cut off after the second term. We take E_o to be 10.2 eV, the energy required to excite hydrogen from the 1s to the 2s state. The expansion is valid for $E < 10.2$ eV, but in this case we must put $k_2 = i\kappa_2$ in Eqs. (45) and (46).

In the triplet case the expansion, Eq. (47), is valid over a fairly long range; however, in the singlet case the presence of a resonance just below the 2s threshold sharply limits the applicability of the expansion. According to the analysis of Ross and Shaw (1961) the effective range approximate formalism can describe only one narrow resonance below threshold. Below this resonance the formalism will not accurately predict the true scattering cross section.

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[7] Ross and Shaw (1961)

Our expansion parameters $M_{ij}(E_o)$ and R_{ij} were obtained by fitting a two term polynomial of the form, Eq. (47), to the computed values of M_{ij} in the range $0 < k_2^2 \leq 1.5 \times 10^{-3}$ Rydbergs. They are given in atomic units in Table III together with the coefficients obtained from the 1s-2s close coupling values by Damburg and Peterkop (1962). In figure 2 the computed NA singlet elastic cross section is compared with our effective range extrapolation. As can be seen, the extrapolation quite accurately reproduces the resonance near $k_1^2 = 0.797$. The second peak at $k_1^2 = 0.735$ is spurious in the present zeroth order problem but more resonances are actually present when relative p-waves are included in the calculation.[8]

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[8] See Gailitis and Damburg (1963) and footnote 6.

Table III

The first two coefficients in the expansion of the M matrix elements at the 2s threshold, eq. (5.3)

NA = nonadiabatic CC = close coupling[a]

	Singlet		Triplet	
	NA	CC	NA	CC
$M_{11}(0)$	1.0610	1.300	0.0293	0.0301
$M_{21}(0)$	-0.0569	-0.0629	-0.0017	-0.0017
$M_{22}(0)$	-0.0368	-0.0356	0.1208	0.1206.
R_{11}	4.2267	4.82	1.1373	1.20
R_{12}	-3.9292	-4.32	0.0642	-0.06
R_{22}	11.489	11.54	5.1528	5.14

[a] Close coupling coefficients taken from Damburg and Peterkop (1962).

Figure 2. Comparison of the computed singlet nonadiabatic (1s-1s) cross section (solid line) near the 2s threshold with effective range extrapolations. Circles are the nonadiabatic effective range extrapolation. Triangles are the (1s-2s) close coupling effective range extrapolation of Damburg and Peterkop (1962). The figure is discussed in the text.

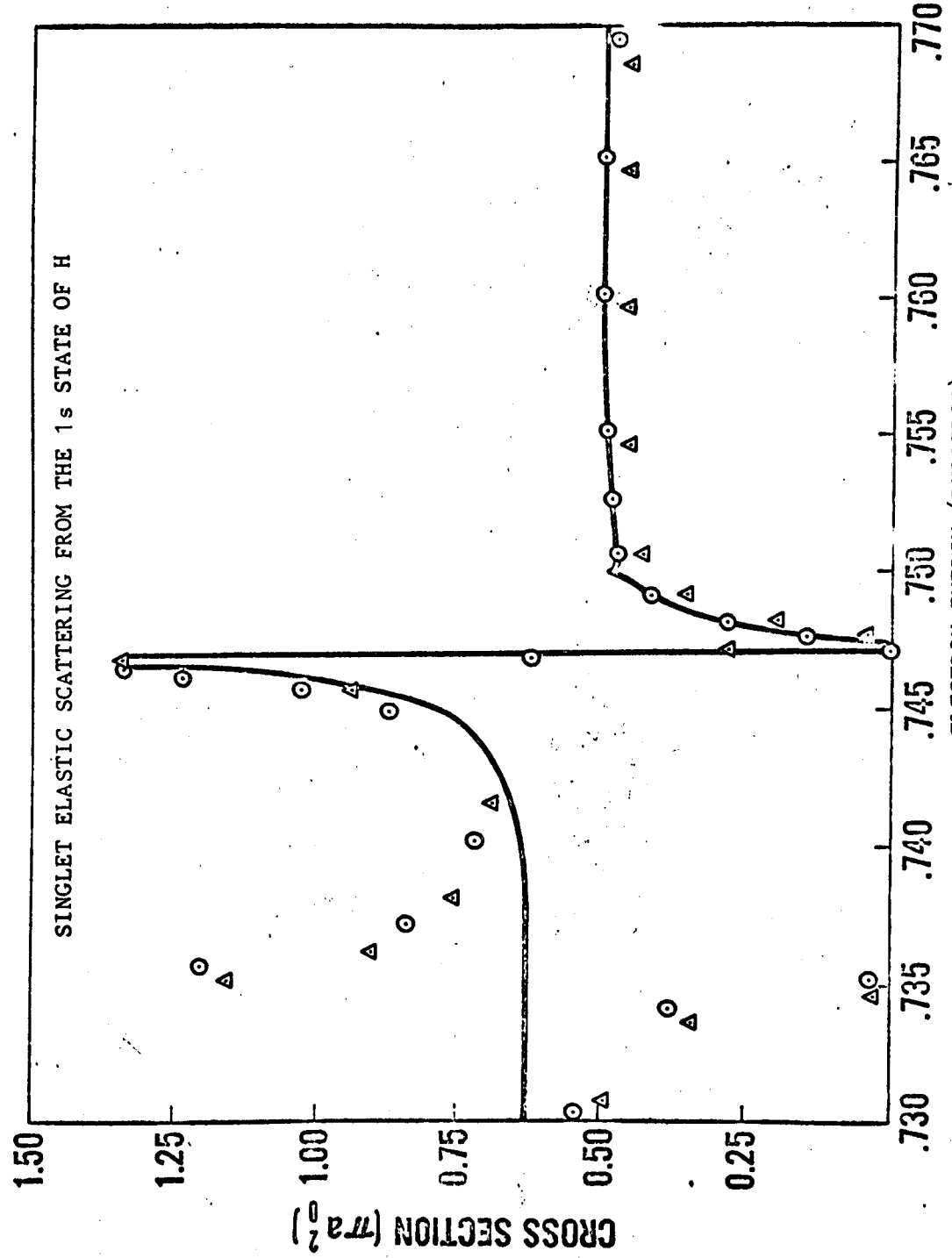
SINGLET ELASTIC SCATTERING FROM THE 1s STATE OF H
CROSS SECTION (πa_0^2)
1.50
1.25
1.00
0.75
0.50
0.25
.730
.735
.740
.745
.750
.755
.760
.765
.770
ELECTRON ENERGY (RYDBERGS)

Figure 2

8. Results

The results obtained from the zeroth order approximation of the $L = 0$ scattering cross sections $\sigma_{1s\text{-}1s}$, $\sigma_{1s\text{-}2s}$, $\sigma_{2s\text{-}2s}$ are shown in Tables IV to VI and in Figures 2 to 5. For comparison purposes the (1s-2s) close coupling results are also given. As previously stated the latter calculation is an approximate variational solution of the zeroth order problem. The internal consistency of our calculations has already been extensively examined in Sec. 6. For the nonadiabatic entries in Tables IV-VI the number of significant figures given indicates the internal consistency of the calculation with the last figure being in doubt. For the singlet entries at $k_1 = 1.5$ even the first significant figure is uncertain. The NA singlet case (i) cross sections are the ones which are plotted in the graphs; however, the case (ii) calculations are of equal weight.

In Figure 3 the nonadiabatic $\sigma_{1s\text{-}2s}$ cross sections are compared with the close coupling expansion with the 1s and 2s channels open. The close coupling results just above threshold were kindly computed for us by Dr. Omidvar of the Theoretical Division of the Goddard Space Flight Center. They appear to be in good agreement with those of Damburg and Peterkop (1962). The other close coupling results were obtained from Marriott (1958) and Omidvar (1964), which in turn are in good agreement with those of Burke and his co-workers (1962, 1963). The nonadiabatic results are about 40 percent lower than those of the close coupling calculation. In fact, the case (i) nonadiabatic $\sigma_{1s\text{-}2s}$ cross sections agree quite well with the variational

calculation of Massey and Moiseiwitsch (1953).

Figure 4 shows the zeroth order nonadiabatic elastic singlet cross section in the neighborhood of the threshold (10.203 eV) and out to 30 eV. A definite Wigner cusp is indicated at threshold. The close coupling results, dashed line, also indicate a cusp at threshold. The plotted case (i) σ_{1s-1s} is only 5 percent larger than the close coupling value at 30 eV. However, the case (i) cross section is about 20 percent larger at this energy.

Our triplet elastic cross sections agree with the close coupling results to better than one percent. Since the triplet cross sections dominate in this region, the total nonadiabatic $\sigma_{1s-1s} = (\sigma_s + \sigma_t)$ lies within two percent of the close coupling result.

In Figure 5 the σ_{2s-2s}, derived in Sec. 5, are shown. Note the Ramsauer minima in the singlet and triplet cross sections. Due to the requirement of conservation of current, σ_{2s-2s} cannot actually go to zero at these minima unless σ_{2s-1s} (and hence σ_{1s-2s}) go to zero also. The narrow minimum in the singlet cross section at 1.87 eV (dashed line) is caused by the presence of the 3s threshold at 1.89 eV. The 3s state must be included in the calculation for this minimum to appear. For this reason the CC calculation does not indicate its presence. The exact shape and depth of this resonance are uncertain due to the scatter of our results and the large I_S obtained inside the resonance. There are undulations of a few percent in the singlet σ_{1s-1s} and σ_{1s-2s} at this point, but the effect is quite small compared to the σ_{2s-2s} resonance. These details in the $L = 0$ portion of

σ_{2s-2s} may well not appear in the total cross section since the CC calculation indicates that the $L = 1$ and the $L = 2$ contributions are very important at the energies where the minima occur.

It would be of interest to be able to solve the zeroth order equation (22) exactly by numerical means. A continuing effort is being made to do this with the noniterative method which has already been used in the triplet case below threshold by Temkin and Sullivan (1963). So far the results have been unsatisfactory. This is at least partly due to the large effective interaction radius between the 2s state of hydrogen and the scattered electron.

Table IV

The spherically symmetric portion of the L = 0 elastic (1s-1s) cross section for the scattering of electrons by atomic hydrogen in units of πa_o^2. NA = Nonadiabatic[a], CC = Close coupling 1s-2s[b].

	Singlet		Triplet		Sum	
k_1(a.u.)	NA	CC	NA	CC	NA	CC
0.810[c]	0.635					
0.863	0.760					
0.864	1.20					
0.26429	1.337					
0.8645	0.0					
0.865	0.2925					
0.8654	0.3893					
0.8656	0.4255					
0.8658	0.4465					
0.866	0.4743					
0.86601	0.4768					
0.86602	0.4795					
0.866025	case(i)	case(ii)		Threshold		
0.86604	0.4790	0.4789				
0.8661	0.4755	0.4754	0.4244	3.995	3.995	4.470	4.4194
0.8662	0.4742	0.4740	0.4235	3.994	3.993	4.468	4.4165
0.870		0.4955	0.4541	3.958	3.957	4.454	4.4111
0.880	0.4955	0.4954	0.4568	3.864	3.864	4.359	4.3208
0.89	0.4826	0.4825	0.4454	3.773	3.772	4.256	4.2174
0.90	0.4674	0.4673	0.4324	3.684	3.684	4.151	4.1164
0.94	0.399	0.399		3.349		3.748	
1.0	0.327	0.330	0.2824	2.905	2.903	3.233	3.1854
1.1	0.239	0.250	0.1865	2.300	2.297	2.550	2.4835
1.2	0.175	0.190	0.1397	1.833	1.829	2.023	1.9687
1.5	0.095	0.113	0.0905	0.974	0.9716	1.087	1.0621

[a] The statistical factors 1/4 and 3/4 are included in the cross sections. When available, case (ii) results were used to find the total scattering cross sections.

[b] All close coupling results were computed by K. Omidvar. Some of these results have not been published, while the rest are taken from Omidvar (1964).

[c] The energy of the incident electron in Rydbergs is just k_1^2.

Table V

The spherically symmetric portion of the $L = 0$ (1s-2s) cross section for the excitation of atomic hydrogen by electrons in units πa_o^2. NA = Nonadiabatic and CC = Close coupling 1s-2s[a].

	Singlet			Triplet		Sum	
	NA		CC	NA	CC	NA	CC
k_1(a.u.)	case(i)	case(ii)					
0.86604	0.0066	0.0066				0.0066	
0.8661	0.0142	0.0142	0.0168	9.9×10^{-6}	9×10^{-6}	0.0142	0.0168
0.8662	0.0204	0.0204	0.0266	1.5×10^{-5}	1.6×10^{-5}	0.0204	0.0266
0.870		0.0354	0.0420	7.8×10^{-5}	8.3×10^{-5}	0.0355	0.0420
0.880	0.0313	0.0314	0.0356	1.8×10^{-4}	1.9×10^{-4}	0.0316	0.0358
0.890	0.0318	0.0319	0.0355	2.7×10^{-4}	2.9×10^{-4}	0.0322	0.0322
0.90	0.0339	0.0338	0.0375	3.8×10^{-4}	4×10^{-4}	0.0342	0.0379
0.94	0.0448	0.0448		9.1×10^{-4}		0.0457	
1.0	0.046	0.048	0.0725	1.9×10^{-3}	2.1×10^{-3}	0.050	0.0746
1.1	0.035	0.040	0.0701	3.3×10^{-3}	4.4×10^{-3}	0.043	0.0745
1.2	0.031	0.039	0.0547	4.7×10^{-3}	6.1×10^{-3}	0.044	0.0608
1.5	0.013	0.019	0.0241	5.6×10^{-3}	7.3×10^{-3}	0.025	0.0314

[a] See footnotes on Table IV

Table VI

The spherically symmetric portion of the L = 0 (2s-2s) cross section for the scattering of electrons by atomic hydrogen in units of πa_0^2. NA = Nonadiabatic and CC = Close coupling 1s-2s[a].

	Singlet			Triplet		Sum	
	NA		CC	NA	CC	NA	CC
k_2(a.u.)	case(i)	case(ii)					
0.00503	654.	654.					
0.0114	622.	622.	650.3	205.0		827.	
0.0174	579.	579.	602.0	204.0	206.8	783.	808.8
0.0831		137.	135.55	170.6	172.3	307.6	307.85
0.1562	19.6	19.6	19.36	110.4	110.5	130.0	129.86
0.2052	3.69	3.68	3.515	71.21	71.20	74.89	74.715
0.245	0.441	0.441	0.3303	45.99	45.94	46.531	46.27
0.365	0.43	0.41		7.37		7.78	
0.500	1.8	1.9	1.532	0.02	0.2102	1.92	1.7422
0.678	1.8	1.8	1.115	1.37	1.36	3.17	2.475
0.831	1.3	1.3	0.8980	2.45	2.112	3.75	3.010
1.225	0.60	0.55	0.5702	1.94	1.811	2.49	2.3812

[a] See footnotes on Table IV

FIGURE CAPTIONS

Figure 3. Comparison of zeroth order nonadiabatic 1s-2s excitation cross sections with the close coupling (1s-2s) results. The figure is discussed in the text.

Figure 4. Comparison of the zeroth order nonadiabatic singlet 1s-1s cross section with the close coupling (1s-2s) expansion. The figure is discussed in the text.

Figure 5. Comparison of the zeroth order nonadiabatic 2s-2s scattering cross sections with the results of the close coupling (1s-2s) expansion. The figure is discussed in the text.

Figure 6. The top four curves represent the total close coupling theoretical and the experimental cross sections for the 1s-2s excitation of H by electron impact. The two lower curves give the $L = 0$ angle independent portion of this cross section. The figure is discussed in Chapter I and in Sec. 9 of Chapter II.

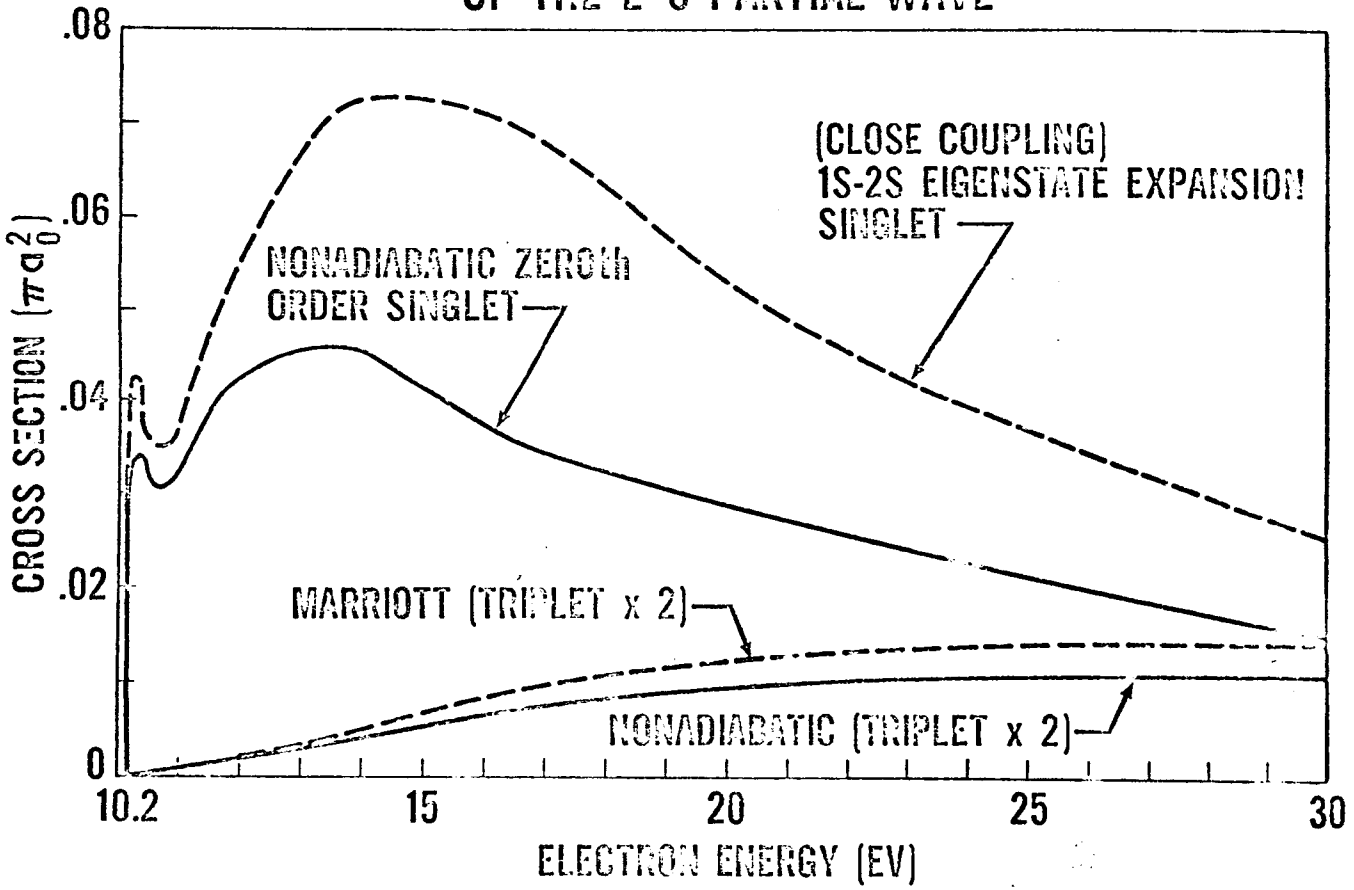
1S-2S EXCITATION CROSS SECTION
USING THE SPHERICAL SYMMETRIC PORTION
OF THE L=0 PARTIAL WAVE
.08
.06
.04
.02
0
CROSS SECTION (πa_0^2)
(CLOSE COUPLING)
1S-2S EIGENSTATE EXPANSION
SINGLET
NONADIABATIC ZEROth
ORDER SINGLET
MARRIOTT (TRIPLET x 2)
NONADIABATIC (TRIPLET x 2)
10.2
15
20
25
30
ELECTRON ENERGY (EV)

Figure 3

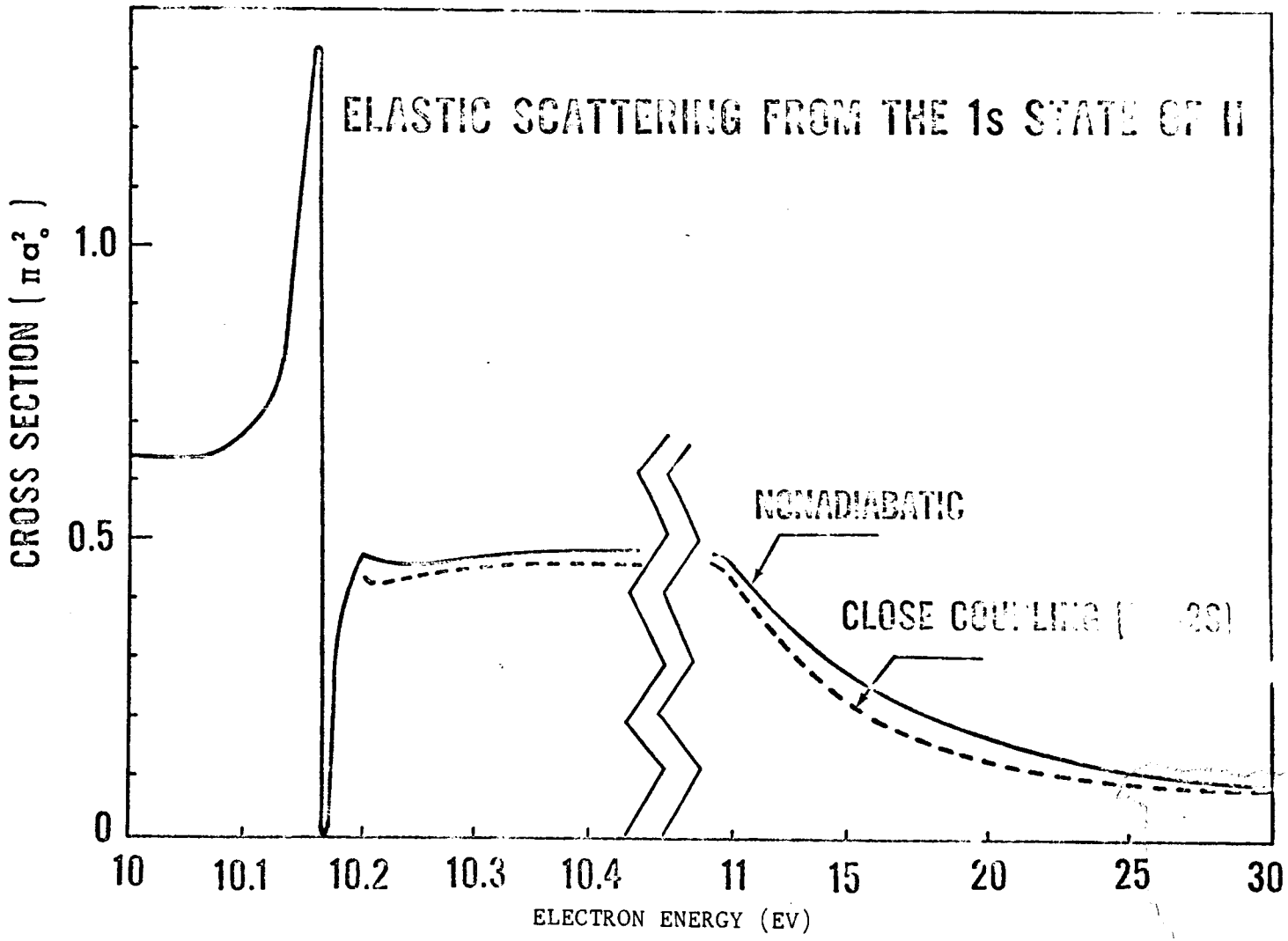
ELASTIC SCATTERING FROM THE 1s STATE OF H
CROSS SECTION (πa_0^2)
1.0
0.5
0
NONADIABATIC
CLOSE COUPLING
10
10.1
10.2
10.3
10.4
11
15
20
25
30
ELECTRON ENERGY (EV)

Figure 4

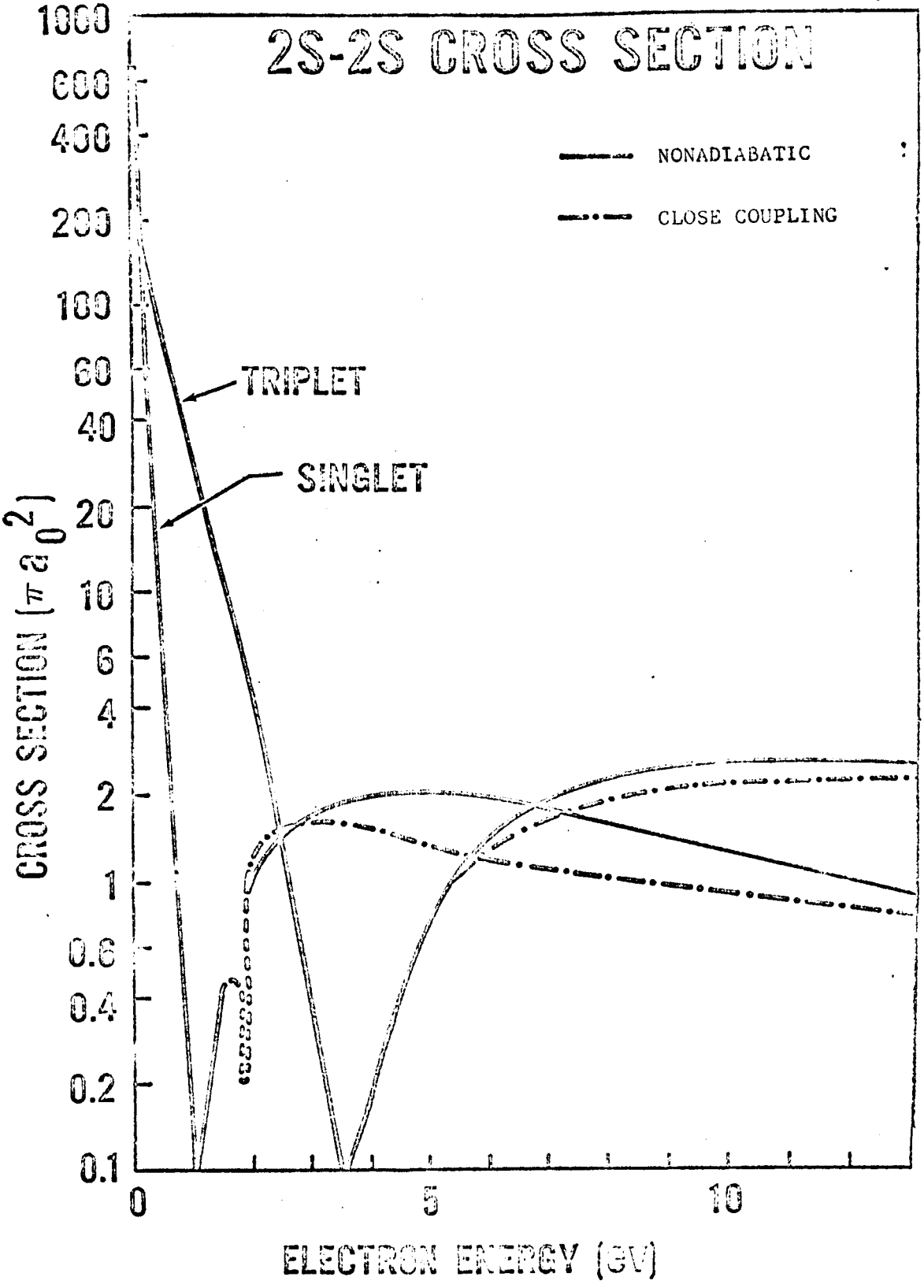
2S-2S CROSS SECTION
NONADIABATIC
CLOSE COUPLING
TRIPLET
SINGLET
CROSS SECTION (πa_0^2)
1000
600
400
200
100
60
40
20
10
6
4
2
1
0.6
0.4
0.2
0.1
0
5
10
ELECTRON ENERGY (eV)

Figure 5

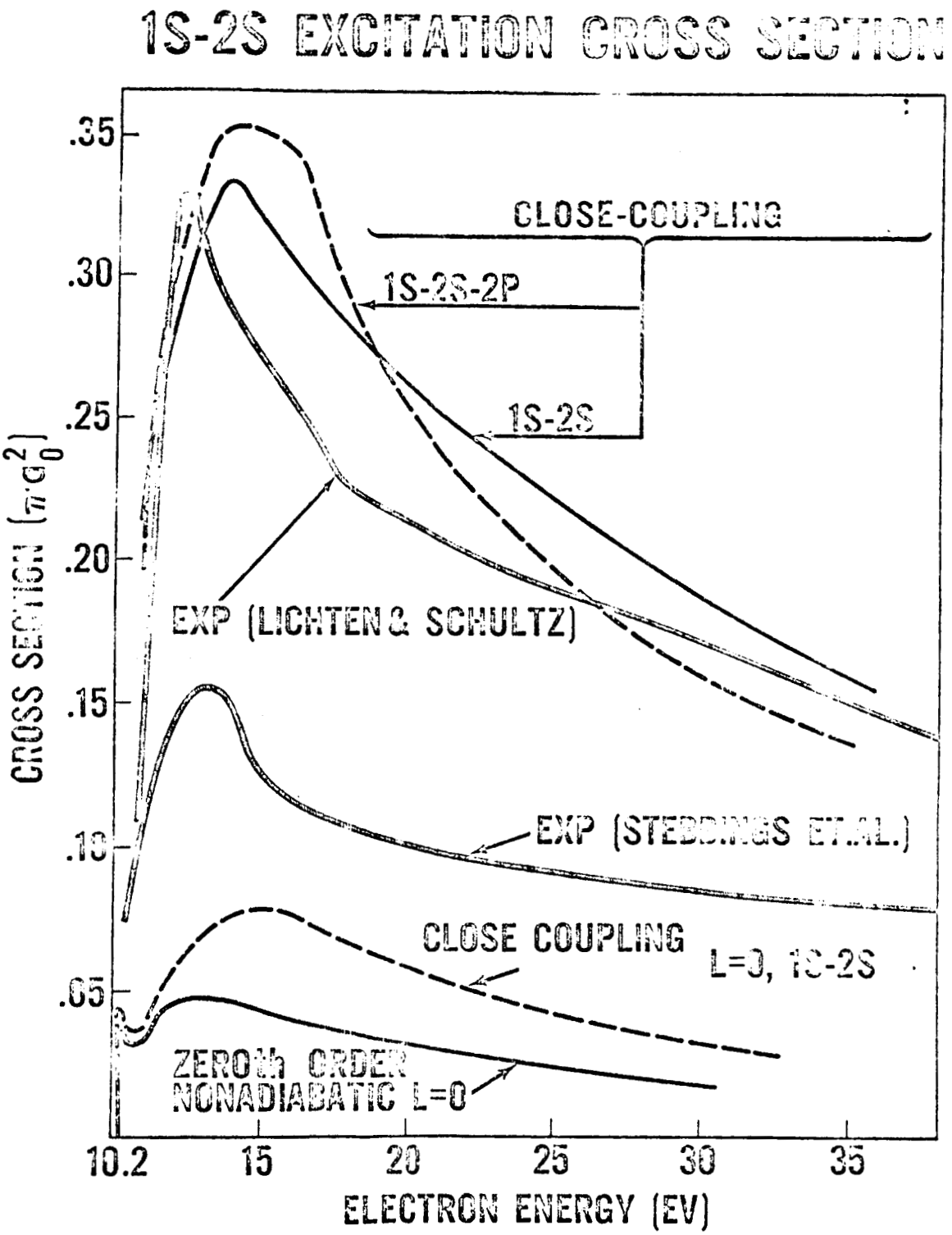
1S-2S EXCITATION CROSS SECTION
CLOSE-COUPLING
1S-2S-2P
1S-2S
EXP (LICHTEN & SCHULTZ)
EXP (STEBBINGS ET.AL.)
CLOSE COUPLING
L=0, 1S-2S
ZEROth ORDER
NONADIABATIC L=0
CROSS SECTION (πa_0^2)
.35
.30
.25
.20
.15
.10
.05
10.2
15
20
25
30
35
ELECTRON ENERGY (EV)

Figure 6

9. Discussion

Figure 6 serves to compare the relative s-wave portion of the $L = 0$ inelastic cross section with the total close coupling theoretical cross section and with the total experimental cross sections obtained by Stebbings et al. (1960) and Lichten and Schultz (1959). Examination of the graph indicates that the zeroth order nonadiabatic $L = 0$, 1s-2s cross section is reduced from the (1s-2s) CC results by about the same percentage as the Lichten and Schultz cross section is reduced from the (1s-2s-2p) CC results around the region of maximum cross section (15 eV), or as the Stebbings et al. measurements are from the Lichten and Schultz results over most of the energy range. Thus this calculation reinforces what one would be tempted to believe on looking at the (1s-2s-2p) CC results in comparison with the experimental results: a more exact theoretical calculation should reduce the theoretical cross section toward the experimental results.

"As to the amount of this decrease one must be infinitely more circumspect in guessing. In the language of the nonadiabatic theory the $L = 0$ part of the 1s-2s-2p calculation refers to the relative s p wave problem whereas the 1s-2s calculation refers to only the relative s-wave problem. From that point of view, the latter appears to be a better approximation relative to its complete solution (to which the present paper is addressed) than the former is to its complete solution. In either case, it might seem ridiculous to try to approximate by two or three terms what in principle is described by a singly or doubly (discrete plus continuous) infinite set of functions. Here, however, one must recall what Seaton (1953) long ago emphasized, that the explicit (anti) symmetrization of the wave function in fact doubles the number of terms and goes a long way in including the effects of the continuum in these calculations. Secondly, with regard to the 1s-2s-2p calculation, the singlet $L = 0$ gives only the second largest contribution to $\sigma_{1s \to 2s}$. The largest contribution comes from the triplet $L = 1$ state. Experience thus far indicates that the close coupling approximation is much more accurate in triplet as opposed to singlet states.

"Thus it is very difficult at this time to infer the correct normalization of the experimental result. In view of the many competing elements which are either included or left out of the close coupling calculation, our own opinion is that the correct normalization of the experimental result is between those of Lichten et al. and Stebbings et al. and closer to the latter, very close, in fact, to that curve where the error bars of the respective experiments overlap (Hummer and Seaton /1961/)."[9]

This conclusion is supported by a recent (1s-2s-2p-3s-3p) close coupling calculation by Taylor and Burke (to be published) which produced more than a 30 percent decrease in $\sigma_{1s\rightarrow 2s}$ at 16.5 eV from the close coupling (1s-2s-2p) calculation.

Additional theoretical and experimental work is desirable on this problem. In particular it is desirable to try to estimate the complete nonadiabatic $L = 0$ cross section and thus obtain a check on the (1s-2s-2p) CC results near threshold. Much more work remains to be done before total nonadiabatic cross sections (sum over-all values of L) can be obtained. In this connection it should also be pointed out that this calculation indicates that the computational error in the nonadiabatic results is large for incident electron energies above 20 eV. Unless this defect can be remedied the usefulness of the nonadiabatic inelastic scattering theory will be somewhat circumscribed.

There will probably be additional close coupling calculations of the total 1s-2s excitation cross section with additional open channels. However, as the work of Taylor and Burke (to be published) indicates, the addition of new channels greatly increases the amount of computer

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[9] Kyle and Temkin (to be published).

time needed for the calculations. This may put a limit to the number of hydrogen wave functions which may be used in the expansion of ψ_4, Eq. (5).

It is to be hoped that more accurate measurements of the absolute 1s-2s excitation cross section will be made in the near future. However, as arguments concerning the Lichten and Schultz experiment demonstrate, the accuracy of final experimental results can be no greater than that of the theory which is used to interpret the actual measurements. Thus it may well be that in this problem theoretical and experimental advances will continue to be strongly interdependent.

Finally it should be pointed out that the results of this calculation, together with those of Damburg and Peterkop (1962), show that one must be very cautious in naively extrapolating cross sections to threshold using the threshold behaviour law stated by Wigner (1948). For the type of problem considered here, Wigner states that near the excitation threshold

$$\sigma_{i\to f} \propto k_f^{2l_f+1} .$$

Here $\sigma_{i\to f}$ is the probability for the target atom being excited from the initial state 'i' to the final state 'f' and l_f is the angular momentum quantum number of the final state. The present results, Table 5, indicate that the law's range can be exceedingly small. Gailitis and Damburg (1963) pointed out that when the 2p state is included in the calculation, the 2s and 2p states are degenerate and hence Wigner's threshold law no longer necessarily applies.

The End

Appendix A

Details of the Case (i) Solution

It will be recalled that $\Phi_o^{(0)}$ is expanded in a series given by Eq. (26),

$$\Phi_o^{(0)}(r_1 r_2) = \left(\frac{A}{k_1}\sin k_1 r_1 + a e^{ik_1 r_1}\right) R_{1s}(r_2) + b e^{ik_2 r_1} R_{2s}(r_2) + \left(\sum_n + \int dp\right) C_n e^{-\kappa_n r_1} R_{ns}(r_2), \tag{26}$$

and that the coefficients a, b, and C_n are to be determined so that I_T (or I_S), Eq. (30), is a minimum. The effort to simulate the sum plus integral in the last term of Eq. (26) was restricted by the fact that the computer could handle no more than eight C_n (see Chap. II, Sec. 6). It was considered best, therefore, to replace the integral by a simple sum,

$$\int C_n e^{-\kappa_n r_1} R_{ns}(r_2)\, dp \rightarrow \sum_{l=1}^{N_1} C_{p_l} e^{-\kappa_{p_l} r_1} U_{p_l}(r_2) . \tag{A-1}$$

An alternate representation of the integral as a sum

$$\int C_n e^{-\kappa_n r_1} R_{ns}(r_2)\, dp \tag{A-2}$$

$$\rightarrow \sum_{l=2}^{N_2} \frac{1}{2}\left\{C_{p_{l-1}} e^{-\kappa_{p_{l-1}} r_1} U_{p_{l-1}}(r_2) + C_{p_l} e^{-\kappa_{p_l} r_1} U_{p_l}(r_2)\right\}(p_l - p_{l-1})$$

was also used. There was no significant difference in the results

obtained from (A-1) and (A-2); however, when (A-2) was used the program was usually restricted to seven C_n due to the added factors $(p_q - p_{q-1})$. Because of this the form (A-1) was generally used. In (A-1) and (A-2) N_2 represents the total number of continuum states included, while $U_p(r)$ is the coulombic s-wave function which obeys the equation

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} + p^2 \right) U_p(r) = 0 . \qquad \text{(A-3)}$$

Consider the triplet case (i) when form (A-1) is used; then I_T takes the explicit form:

$$I_T = \int_0^\infty \left| \Phi_0^{(0)}(r_1 r_2) \right|^2_{r_1 = r_2} dr \qquad \text{(A-4)}$$

$$= \tfrac{1}{2}(1 + X^2 + 2\alpha^2 Z^2 + Z^4) + \tfrac{1}{2}(X^2 + Z^4 - 1)\eta_{2C}$$

$$+ X\eta_{2S} + 2\alpha Z\left[(\eta_+ + \xi_+ X + \eta Z^2)\cos\delta + (\xi_- - \eta X + \xi_+ Z^2)\sin\delta\right]$$

$$+ 2\sum_{n=1}^{N} \left\{ \gamma_n I_{p_n 1S} + (X\gamma_n + \epsilon_n Z^2) I_{p_n 1C} \right.$$

$$\left. + \alpha Z\left[(\gamma_n I_{p_n 2C} + \epsilon_n I_{p_n 2S})\cos\delta - (\gamma_n I_{p_n 2S} - \epsilon_n I_{p_n 2C})\sin\delta\right] \right\}$$

$$+ \sum_{n=1}^{N}\sum_{m=1}^{N} (\gamma_n \gamma_m + \epsilon_n \epsilon_m)(ME)_{p_n p_m} .$$

Here the C_n are given the form

$$C_n = \gamma_n + i\epsilon_n \quad . \tag{A-5}$$

Let N_1 be the number of discrete virtual states, then the total number of discrete plus continuum virtual states is $N = N_1 + N_2$. The coefficients χ, ξ, and δ, Eq. (34), and the γ_n and ϵ_n are to be determined by Eq. (29). The other quantities in (A-4) are defined below.

$$\left.\begin{aligned}
&\alpha = (k_1/k_2)^{1/2} \\
&\begin{pmatrix}\eta_{2s}\\ \eta_{2c}\end{pmatrix} = \int_0^\infty \begin{pmatrix}\sin 2k_1 r\\ \cos 2k_1 r\end{pmatrix} R_{1S}^2(r)\,dr \\
&\zeta_\pm = \int_0^\infty \{\cos(k_1+k_2)r \pm \cos(k_1-k_2)r\} R_{1S}(r) R_{2S}(r)\,dr \\
&\eta_\pm = \int_0^\infty \{\sin(k_1+k_2)r \pm \sin(k_1-k_2)r\} R_{1S}(r) R_{2S}(r)\,dr
\end{aligned}\right\} \tag{A-6}$$

For $n \le N_1$ the integrals

$$\begin{pmatrix} I_{p_n ms} \\ I_{p_n mc}\end{pmatrix} \rightarrow \begin{pmatrix} I_{n,ms} \\ I_{n,mc}\end{pmatrix} \tag{A-7}$$

$$= \int_0^\infty \begin{pmatrix}\sin k_m r\\ \cos k_m r\end{pmatrix} e^{-\chi_n r} R_{ms}(r) R_{ns}(r)$$

where $m = 1, 2$ and $n \ge 3$.

If also $\ell \leq N_1$ then:

$$(ME)_{p_n p_\ell} \rightarrow (ME)_{n,\ell} = \int_0^\infty e^{-(\kappa_n + \kappa_\ell)r} R_{ns}(r) R_{\ell s}(r)\, dr \tag{A-8}$$

The integrals (A-6) -- (A-8) may be evaluated easily if one uses any standard table of integrals and recalls that $R_{ns}(r)$ is just r times the nth radial s-wave function of atomic hydrogen.

The remaining integrals (A-9, A-10, A-11) are given in Appendix B.

$$\begin{pmatrix} I_{p_n ms} \\ I_{p_n mc} \end{pmatrix} = \int_0^\infty \begin{pmatrix} \sin k_m r \\ \cos k_m r \end{pmatrix} e^{-\kappa_{p_n} r} R_{ms}(r) U_{p_n}(r)\, dr \tag{A-9}$$

$m = 1, 2$ and $n > N_1$,

$$(ME)_{p_n p_\ell} \rightarrow (mE)_{n p_\ell} = \int_0^\infty e^{-(\kappa_n + \kappa_{p_\ell})r} R_{ns}(r) U_{p_\ell}(r)\, dr \tag{A-10}$$

$n \leq N_1$ and $\ell > N_1$,

$$(ME)_{p_n p_\ell} = \int_0^\infty e^{-(\kappa_{p_n} + \kappa_{p_\ell})r} U_{p_n}(r) U_{p_\ell}(r)\, dr \tag{A-11}$$

$n > N_1$ and $\ell > N_1$.

The γ_n and ϵ_n may be expressed in terms of X, z, and δ by use of Eq. (29). The equation

$$\partial I_T / \partial \gamma_n = 0 \tag{A-12}$$

actually stands for a set of N equations linear in the γ_n. Similarly

$$\partial I_T / \partial \epsilon_n = 0 \tag{A-13}$$

stands for N equations linear in the ϵ_n. These two sets of equations yield

$$\gamma_n = S_1(n) + S_2(n) X + \alpha z \left(S_3(n) \cos\delta - S_4(n) \sin\delta \right) \tag{A-14}$$

and

$$\epsilon_n = S_1(n) z^2 + \alpha z \left(S_3(n) \sin\delta + S_4(n) \cos\delta \right) \tag{A-15}$$

where

$$S_j(n) = -D_j^{(n)} / \det \qquad j = 1, 4. \tag{A-16}$$

Here det is the determinant of the matrix

$$\begin{pmatrix} (ME)_{p_1 p_1} & (ME)_{p_1 p_2} & \cdots & (ME)_{p_1 p_N} \\ \cdot & \cdot & & \cdot \\ \cdot\cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ (ME)_{p_N p_1} & (ME)_{p_N p_2} & \cdots & (ME)_{p_N p_N} \end{pmatrix} \tag{A-17}$$

and the $D_j^{(n)}$ are the determinants obtained by replacing the nth column of the above matrix with the column vector:

$$j = 1 \quad (I_{p_1 1s} \cdots I_{p_n 1s})$$

$$j = 2 \quad (I_{p_1 1c} \cdots I_{p_n 1c})$$

$$j = 3 \quad (I_{p_1 2c} \cdots I_{p_n 2c})$$

$$j = 4 \quad (I_{p_1 2s} \cdots I_{p_n 2s}) .$$

The equation

$$\partial I_T / \partial X = 0 \tag{A-18}$$

is linear in x and yields

$$X = - W_1/W_2 - \alpha z \left(\frac{W_3}{W_2} \cos\delta - \frac{W_4}{W_2} \sin\delta \right) \tag{A-19}$$

where

$$\left.\begin{aligned} W_1 &= \eta_{2s} + 2 \sum_n I_{p_n 1c} S_1(n) \\ W_2 &= (1+\eta_{2c}) + 2 \sum_n I_{p_n 1c} S_2(n) \\ W_3 &= \beta_+ + 2 \sum_n S_3(n) I_{p_n 1c} \\ W_4 &= \eta_- + 2 \sum_n I_{p_n 1c} S_4(n) . \end{aligned}\right\} \tag{A-20}$$

Next note that

$$\partial I_T / \partial \delta = 0 \tag{A-21}$$

is quadratic in z. When (A-21) is solved for $z(\delta)$ one obtains

$$z = \{ -A_2 \pm (A_2^2 - 4 A_1 A_3)^{1/2} \} / 2 A_3 \tag{A-22}$$

where $A_1 = A_{1a}\cos(\delta) - A_{1b}\sin(\delta)$

$$A_2 = A_{2a} + A_{2b}\cos(2\delta) + A_{2c}\sin(2\delta)$$

$$A_3 = A_{3a}\cos(\delta) - A_{3b}\sin(\delta)$$

and

$$A_{1a} = \xi_+ + 2\sum_n I_{p_n 2c}\, S_2(n)$$

$$A_{1b} = \eta_- + 2\sum_n I_{p_n 2s}\, S_2(n)$$

$$A_{2a} = \alpha(W_3 R_2 - W_4 R_1)/2W_2 + 2\alpha\sum_n \left(S_4(n) I_{p_n 2c} - S_3(n) I_{p_n 2s}\right)$$

$$A_{2b} = \alpha(W_3 R_2 + W_4 R_1)/2W_2$$

$$A_{2c} = \alpha(W_3 R_1 - W_4 R_2)/2W_2$$

$$A_{3a} = \xi_- + W_1 R_2/W_2 - 2\sum_n S_1(n) I_{p_n 2c}$$

$$A_{3b} = \eta_+ - W_1 R_1/W_2 + 2\sum_n S_1(n) I_{p_n 2c}$$

$$R_1 = \xi_+ + 2\sum_n S_2(n) I_{p_n 2c}$$

$$R_2 = \eta_- + 2\sum_n S_2(n) I_{p_n 2s}$$

At this point all the coefficients X, Z, γ_n and ϵ_n are expressed as functions of δ. In order to determine the value of δ which will minimize I_T, let

$$W_\delta = \partial I_T/\partial Z \qquad \text{(A-23)}$$

Then the zeros of Wq will correspond to the extrema of I_T. The zeros of Wq were found by programming the equations given above on the computer and sweeping δ from 0 to 2π. Two identical minima of I_T were found; one for $0 \leq \delta < \pi$ and one for $\pi \leq \delta < 2\pi$. The minima in I_T and I_S were very sharp and a mesh size of $\Delta\delta = \pi/10{,}000$ was sometimes needed just to find them. As a rule $\sigma_{1s\text{-}2s}$ varied with (δ) so rapidly near the minimum of I_T (or I_S) that the accuracy of $\sigma_{1s\text{-}2s}$ would have been restricted to three or four significant figures even if no other difficulties had occurred (see Chap. II, Sec. 6). On the other hand, $\sigma_{1s\text{-}1s}$ varied slowly near the minimum in I_T (or I_S) and could therefore be determined with much greater accuracy.

The solution of the singlet case (i) problem is completely analogous to that of the triplet. In fact, if the terms in I_S are grouped properly, much of the triplet machine program may also be used in the singlet case. Define

$$\left.\begin{aligned}
\begin{pmatrix} f_1(r) \\ f_2(r) \end{pmatrix} &= \begin{pmatrix} Re \\ Im \end{pmatrix} \left\{ \left(-\frac{\partial}{\partial r_1} + \frac{\partial}{\partial r_2}\right) \left[\sin k_1 r_1 + i \cos k_1 r_1 \right] R_{1s}(r_2) \right\}_{r_1 = r_2} \\
\begin{pmatrix} f_3(r) \\ f_4(r) \end{pmatrix} &= \begin{pmatrix} Re \\ Im \end{pmatrix} \left\{ \left(-\frac{\partial}{\partial r_1} + \frac{\partial}{\partial r_2}\right) \left[e^{i k_2 r_1} R_{2s}(r_2) \right] \right\}_{r_1 = r_2} \\
V_{p_n}(r) &= \left\{ \left(-\frac{\partial}{\partial r_1} + \frac{\partial}{\partial r_2}\right) \left(e^{-\kappa_{p_n} r_1} U_{p_n}(r_2) \right) \right\}_{r_1 = r_2}
\end{aligned}\right\} \quad \text{(A-24)}$$

Then

$$S\eta_{\pm} = \frac{1}{2}\int_0^{\infty} \begin{pmatrix} f_1 f_3 \\ f_2 f_4 \end{pmatrix} dr \quad ; \quad S\zeta_{\pm}^{\rho} = \frac{1}{2}\int_0^{\infty} \begin{pmatrix} f_2 f_3 \\ -f_1 f_4 \end{pmatrix} dr \tag{A-25}$$

$$\left.\begin{aligned} SI_{\rho_n 1S} &= \int_0^{\infty} f_1 V_{\rho_n} dr \quad ; SI_{\rho_n 1C} = \int_0^{\infty} f_2 V_{\rho_n} dr \\ SI_{\rho_n 2C} &= \int_0^{\infty} f_3 V_{\rho_n} dr \quad ; SI_{\rho_n 2S} = \int_0^{\infty} f_4 V_{\rho_n} dr \end{aligned}\right\} \tag{A-26}$$

and

$$(SME)_{\rho_\ell \rho_m} = \int_0^{\infty} V_{\rho_\ell} V_{\rho_n} dr \tag{A-27}$$

If one uses these definitions, the equations (A-14) to (A-23) may be used in the singlet solution with only minor changes in the definition of certain terms.

When case (ii), Eq. (35), is considered, the problem becomes much more difficult from the computational viewpoint. The case (ii) solution is very similar to that of case (i) through Eq. (A-20). One is able to solve for $x = x(\delta_1, \delta_2)$, but the equations for the scattering phase shifts δ_1 and δ_2 have to be solved numerically by sweeping δ_1 and δ_2 from $0 \rightarrow 2\pi$. Because of this a case (ii) run required about twenty times as much computer time and about ten times as much of the programmer's time as a case (i) run.

Appendix B

Integrals Involving $U_p(r)$, the Continuum Coulomb Wave Function[1]

"All formulas are obtainable from the very general formulas of Alder et al. (1956). The results involve, among others, the various kinds of hypergeometric . . . functions. The notation for these is standard aside from minor variations. Definitions may be found in innumerable books; we mention only Morse and Feshback (1953). Many of the formulas are not manifestly real; nevertheless, they may all be shown to be real. Those matrix elements which should be symmetric with respect to the interchange of initial and final states can be shown to be symmetric. The reality and symmetry are, in fact, closely related.

"The continuum coulomb functions are normalized as follows:

$$U_p(r) = r e^{-ipr} F(1 + i/p; 2; 2ipr) \cdots$$

$F(a;b;x)$ is the confluent hypergeometric function . . . For the purpose of giving the discrete continuum matrix elements, it is convenient to write the discrete wave functions in the form

$$R_{ns}(r) = e^{-r/n} \sum_{j=1}^{n} C_{nj} r^j$$

where C_{nj} is the coefficient of r^j in

$$R_{ns}(r) = (n)^{-1/2} (2rn^{-1}) e^{-r/n} F(-n+1; 2; 2rn^{-1})$$." [1]

The integrals given here were checked by numerical integration. To insure that the poles in the complex integrals were placed in the correct quadrant it was found advisable to use two arctangent functions in the machine program. The first ($\tan^{-1}$) had a range from $-\pi/2$ to $\pi/2$, while the second (Atan) had a range from 0 to 2π.

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[1] This appendix is very similar to the appendix in Temkin (1962A). The quote and a number of the integrals are taken directly from this source.

Triplet formulas:

$$(ME)_{p_1 p_2} = \{ [2\lambda \exp(\tfrac{p_1 - p_2}{p_1 p_2} \tan^{-1}\tfrac{(p_1 - p_2)}{\lambda} - \tfrac{p_1 + p_2}{p_1 p_2} \tan^{-1}\tfrac{(p_1 + p_2)}{\lambda}$$

$$+ i \tfrac{(p_2 - p_1)}{2 p_1 p_2} \ln\left(\tfrac{\lambda^2 + (p_1 - p_2)^2}{\lambda^2 + (p_1 + p_2)^2} \right))] / [\lambda^2 + (p_1 - p_2)^2][\lambda^2 + (p_1 + p_2)^2] \}$$

$$\times \{ F(-ip_2^{-1}, ip_1^{-1}; 1; x) - \tfrac{2y[\lambda + i(p_1 - p_2)]}{\lambda^2 + (p_1 - p_2)^2} F(1 - ip_2^{-1}, 1 + ip_1^{-1}; 2; x) \},$$

where F(a,b;c;x) are hypergeometric functions, $\lambda = \kappa_{p_1} + \kappa_{p_2}$

$x = 4p_1p_2/[\lambda^2 + (p_1 + p_2)^2]$, and $y = 1-x$.

$$(ME)_{n,p} = \sum_{j=1}^{n} C_{nj} \mathcal{J}_j(\lambda_{np})$$

where $\lambda_{np} = \kappa_n + \kappa_p + n^{-1}$, $\qquad \mathcal{J}_j(\lambda) = \int_0^\infty e^{-\lambda r} r^j U_p(r) dr.$

Hence $\mathcal{J}_j(\lambda) = -(\partial/\partial\lambda)\mathcal{J}_{j-1}(\lambda)$, and

$$\mathcal{J}_0(\lambda) = \left(\frac{\lambda + ip}{\lambda - ip}\right)^{i/p} \left(\frac{1}{\lambda^2 + p^2}\right)$$

$$= (\lambda^2 + p^2)^{-1} \exp[-2p^{-1} \tan^{-1}(p/\lambda)].$$

The integrals $\mathcal{J}_j(\lambda)$ may also be used to derive the matrix elements $I_{pm(\ell)}$.

Define:

$$\begin{pmatrix} J_{pjc}(k_m) \\ J_{pjs}(k_m) \end{pmatrix} = \int_0^\infty \begin{pmatrix} \cos k_m r \\ \sin k_m r \end{pmatrix} e^{-\lambda_m r} r^j U_p(r)\, dr$$

$$= \begin{pmatrix} R_e \\ \Im_m \end{pmatrix} \int_0^\infty e^{-(\lambda_m + i k_m) r} r^j U_p(r)\, dr$$

$$= T_j(\lambda_m) \left\{ \begin{matrix} \cos \\ \sin \end{matrix} [\theta_j(\lambda_m)] \right\}$$

where $\lambda_m = m^{-1} + \chi_p$; $m = 1, 2$; and

$$T_0(\lambda) = [(\lambda^2 + p^2 - k^2)^2 + (2\lambda k)^2]^{-1/2} \exp\left[-\frac{1}{p}\left(\tan^{-1}\frac{p-k}{\lambda} + \tan^{-1}\frac{p+k}{\lambda}\right)\right]$$

$$\theta_0(\lambda) = \frac{1}{2p} \ln\left[\frac{\lambda^2 + (p-k)^2}{\lambda^2 + (p+k)^2}\right] + \operatorname{atan}\left(\frac{2\lambda k}{\lambda^2 + p^2 - k^2}\right)$$

$$T_1(\lambda) = \frac{2[(\lambda-1)^2 + k^2]^{1/2}}{(p^2 + \lambda^2 - k^2)^2 + (2\lambda k)^2} \exp\left[-\frac{1}{p}\left(\tan^{-1}\frac{p-k}{\lambda} + \tan^{-1}\frac{p+k}{\lambda}\right)\right]$$

$$\theta_1(\lambda) = \frac{1}{2p} \ln\left[\frac{\lambda^2 + (p-k)^2}{\lambda^2 + (p+k)^2}\right] - \operatorname{atan}\frac{k}{\lambda - 1} + 2\operatorname{atan}\frac{2\lambda k}{p^2 + \lambda^2 - k^2}$$

$$T_2(\lambda) = \left\{\frac{2[(3\lambda^2 - 3k^2 - p^2 - 6\lambda + 2)^2 + 36k^2(\lambda-1)^2]^{1/2}}{[(\lambda^2 - k^2 + p^2)^2 + 4\lambda^2 k^2]^{3/2}}\right\}$$

$$\times \exp\left\{-\frac{1}{p}\left[\tan^{-1}\frac{p-k}{\lambda} + \tan^{-1}\frac{p+k}{\lambda}\right]\right\}$$

$$\theta_2(\lambda) = \frac{1}{2p}\ln\left[\frac{\lambda^2+(p-k)^2}{\lambda^2+(p+k)^2}\right] - a\tan\left[\frac{6k(\lambda-1)}{3\lambda^2-3k^2-p^2-6\lambda+2}\right]$$
$$+3a\tan\left[\frac{2\lambda k}{\lambda^2-k^2+p^2}\right].$$

Then $I_{p_1 C} = 2J_{p_1 C}(k_1)\ ;\ I_{p_1 S} = 2J_{p_1 S}(k_1)$,

and $I_{p_1 2(S)} = 2^{-3/2}\left[2J_{p_1 1(S)}(k_2) - J_{p_1 2(S)}(k_2)\right]$.

Singlet formulas (the symbols have the same meaning as the corresponding triplet formulas):

$$(SME)_{p_1 p_2} = \left[2\kappa_{p_1}\kappa_{p_2} + p^2 + \kappa_{p_2}^2 + \lambda^{-1}\kappa_{p_1}(\lambda^2+p_1^2-p_2^2)\right](ME)_{p_1 p_2}$$
$$+2\exp\left\{\frac{p_1-p_2}{p_1 p_2}\tan^{-1}\left(\frac{p_1-p_2}{\lambda}\right) - \frac{p_1+p_2}{p_1 p_2}\tan^{-1}\left(\frac{p_1+p_2}{\lambda}\right)\right.$$
$$\left.+\frac{i(p_2-p_1)}{2p_1 p_2}\ln Y\right\}\frac{F(1-ip_2^{-1}, 1+ip_1^{-1}; 2; X)}{\lambda^2+(p_1+p_2)^2},$$

$$(SME)_{n1p} = (\kappa_n - n^{-1})\sum_{j=1}^{n} C_{nj}\left\{(\kappa_n+\lambda_{np})\mathcal{J}_j(\lambda_{np}) - j\mathcal{J}_{j-1}(\lambda_{np})\right\}$$
$$+\sum_{j=1}^{n} C_{nj}\, j\left\{(\kappa_n+\lambda_{np})\mathcal{J}_{j-1}(\lambda_{np}) - (j-1)\mathcal{J}_{j-2}(\lambda_{np})\right\},$$

$$SI_{p1S} = 2\left\{(\kappa_p+\lambda_1+1)J_{p1S}(k_1) - (\kappa_p+\lambda_1+k_1^2)J_{p1S}(k_1)\right.$$
$$\left.-k_1(\kappa_p+\lambda_1-1)J_{p1C}(k_1)\right\},$$

$$SI_{p1C} = 2\left\{(\kappa_p+\lambda_1+1)J_{p0C}(k_1)-(\kappa_p+\lambda_1+k_1^2)J_{p1C}(k_1)\right.$$
$$\left.+k_1(\kappa_p+\lambda_1-1)J_{p1S}(k_1)\right\},$$

$$SI_{p2S} = 2^{-3/2}\left\{-(2\kappa_p+2\lambda_2+3)J_{p0S}(k_2)+(3\kappa_p+3\lambda_2+2k_2^2+1)J_{p1S}(k_2)\right.$$
$$-\tfrac{1}{2}(\kappa_p+\lambda_2+2k_2^2)J_{p2S}(k_2)+k_2(2\kappa_p+2\lambda_2-1)J_{p1C}(k_2)$$
$$\left.-k_2(\kappa_p+\lambda_2-\tfrac{1}{2})J_{p2C}(k_2)\right\},$$

$$SI_{p2C} = 2^{-3/2}\left\{(2\kappa_p+2\lambda_2+3)J_{p0C}(k_2)-(3\kappa_p+3\lambda_2+2k_2^2+1)J_{p1C}(k_2)\right.$$
$$+\tfrac{1}{2}(\kappa_p+\lambda_2+2k_2^2)J_{p2C}(k_2)+k_2(2\kappa_p+2\lambda_2-1)J_{p1S}(k_2)$$
$$\left.-k_2(\kappa_p+\lambda_2-\tfrac{1}{2})J_{p2S}(k_2)\right\}.$$

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